Johan Ãqvist

List of Publications by Year
in descending order

184	12,882	26630	26613
papers	citations	56 h-index	107 g-index

188	188	188	9959
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ion-water interaction potentials derived from free energy perturbation simulations. The Journal of Physical Chemistry, 1990, 94, 8021-8024.	2.9	1,527
2	A new method for predicting binding affinity in computer-aided drug design. Protein Engineering, Design and Selection, 1994, 7, 385-391.	2.1	1,064
3	Simulation of enzyme reactions using valence bond force fields and other hybrid quantum/classical approaches. Chemical Reviews, 1993, 93, 2523-2544.	47.7	797
4	Ion permeation mechanism of the potassium channel. Nature, 2000, 404, 881-884.	27.8	418
5	Ligand binding affinity prediction by linear interaction energy methods. Journal of Computer-Aided Molecular Design, 1998, 12, 27-35.	2.9	401
6	Ligand Binding Affinities from MD Simulations. Accounts of Chemical Research, 2002, 35, 358-365.	15.6	348
7	Q: a molecular dynamics program for free energy calculations and empirical valence bond simulations in biomolecular systems. Journal of Molecular Graphics and Modelling, 1998, 16, 213-225.	2.4	291
8	Molecular dynamics simulations of water and biomolecules with a Monte Carlo constant pressure algorithm. Chemical Physics Letters, 2004, 384, 288-294.	2.6	277
9	On the Validity of Electrostatic Linear Response in Polar Solvents. The Journal of Physical Chemistry, 1996, 100, 9512-9521.	2.9	270
10	Free Energy Calculations and Ligand Binding. Advances in Protein Chemistry, 2003, 66, 123-158.	4.4	177
11	Mechanism of peptide bond synthesis on the ribosome. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 12395-12400.	7.1	171
12	Cyclic HIV-1 Protease Inhibitors Derived from Mannitol:Â Synthesis, Inhibitory Potencies, and Computational Predictions of Binding Affinities. Journal of Medicinal Chemistry, 1997, 40, 885-897.	6.4	158
13	The Linear Interaction Energy Method for Predicting Ligand Binding Free Energies. Combinatorial Chemistry and High Throughput Screening, 2001, 4, 613-626.	1.1	156
14	Force Field Independent Metal Parameters Using a Nonbonded Dummy Model. Journal of Physical Chemistry B, 2014, 118, 4351-4362.	2.6	148
15	Calculation of absolute binding free energies for charged ligands and effects of long-range electrostatic interactions. Journal of Computational Chemistry, 1996, 17, 1587-1597.	3.3	146
16	Estimation of binding free energies for HIV proteinase inhibitors by molecular dynamics simulations. Protein Engineering, Design and Selection, 1995, 8, 1137-1144.	2.1	142
17	Mechanistic alternatives in phosphate monoester hydrolysis: What conclusions can be drawn from available experimental data?. Chemistry and Biology, 1999, 6, R71-R80.	6.0	138
18	Absolute and Relative Entropies from Computer Simulation with Applications to Ligand Binding. Journal of Physical Chemistry B, 2005, 109, 6448-6456.	2.6	130

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19	pH-sensitivity of the ribosomal peptidyl transfer reaction dependent on the identity of the A-site aminoacyl-tRNA. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 79-84.	7.1	127
20	Binding affinity prediction with different force fields: Examination of the linear interaction energy method. Journal of Computational Chemistry, 2004, 25, 1242-1254.	3.3	125
21	Computer simulation of the initial proton transfer step in human carbonic anhydrase I. Journal of Molecular Biology, 1992, 224, 7-14.	4.2	118
22	Improving the Accuracy of the Linear Interaction Energy Method for Solvation Free Energies. Journal of Chemical Theory and Computation, 2007, 3, 2162-2175.	5.3	112
23	Potent Inhibitors of the Plasmodium falciparum Enzymes Plasmepsin I and II Devoid of Cathepsin D Inhibitory Activity. Journal of Medicinal Chemistry, 2004, 47, 110-122.	6.4	107
24	Exploring blocker binding to a homology model of the open hERG K+channel using docking and molecular dynamics methods. FEBS Letters, 2005, 579, 2939-2944.	2.8	103
25	K+/Na+ selectivity of the KcsA potassium channel from microscopic free energy perturbation calculations. BBA - Proteins and Proteomics, 2001, 1548, 194-202.	2.1	100
26	Entropy and Enzyme Catalysis. Accounts of Chemical Research, 2017, 50, 199-207.	15.6	96
27	Resolving Apparent Conflicts between Theoretical and Experimental Models of Phosphate Monoester Hydrolysis. Journal of the American Chemical Society, 2015, 137, 1081-1093.	13.7	92
28	Cold Adaptation of Enzyme Reaction Rates. Biochemistry, 2008, 47, 10049-10057.	2.5	90
29	Analysis of Predictions for the Catalytic Mechanism of Ribosomal Peptidyl Transferâ€. Biochemistry, 2006, 45, 7049-7056.	2.5	89
30	The catalytic mechanism of protein tyrosine phosphatases revisited. FEBS Letters, 2001, 498, 208-213.	2.8	87
31	Design, Synthesis, Computational Prediction, and Biological Evaluation of Ester Soft Drugs as Inhibitors of Dihydrofolate Reductase fromPneumocystis carinii. Journal of Medicinal Chemistry, 2001, 44, 2391-2402.	6.4	86
32	A Model for How Ribosomal Release Factors Induce Peptidyl-tRNA Cleavage in Termination of Protein Synthesis. Molecular Cell, 2007, 27, 758-766.	9.7	80
33	Catalysis and Linear Free Energy Relationships in Aspartic Proteasesâ€. Biochemistry, 2006, 45, 7709-7723.	2.5	79
34	Combining Docking, Molecular Dynamics and the Linear Interaction Energy Method to Predict Binding Modes and Affinities for Non-nucleoside Inhibitors to HIV-1 Reverse Transcriptase. Journal of Medicinal Chemistry, 2008, 51, 2648-2656.	6.4	79
35	Mechanisms of tetraethylammonium ion block in the KcsA potassium channel. FEBS Letters, 2001, 495, 191-196.	2.8	78
36	Linear Interaction Energy: Method and Applications in Drug Design. Methods in Molecular Biology, 2012, 819, 305-323.	0.9	78

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37	Energetics of nucleophile activation in a protein tyrosine phosphatase. Journal of Molecular Biology, 1997, 265, 118-127.	4.2	77
38	Structures of Mycobacterium tuberculosis 1-Deoxy-D-xylulose-5-phosphate Reductoisomerase Provide New Insights into Catalysis. Journal of Biological Chemistry, 2007, 282, 19905-19916.	3.4	77
39	Computation of enzyme cold adaptation. Nature Reviews Chemistry, 2017, 1, .	30.2	75
40	Enzyme surface rigidity tunes the temperature dependence of catalytic rates. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 7822-7827.	7.1	74
41	Virtual screening and bioassay study of novel inhibitors for dengue virus mRNA cap (nucleoside-2â€²O)-methyltransferase. Bioorganic and Medicinal Chemistry, 2007, 15, 7795-7802.	3.0	72
42	Computer Simulation of the Triosephosphate Isomerase Catalyzed Reaction. Journal of Biological Chemistry, 1996, 271, 10010-10016.	3.4	71
43	A computational study of ion binding and protonation states in the KcsA potassium channel. BBA - Proteins and Proteomics, 2000, 1481, 360-370.	2.1	71
44	Calculations of solute and solvent entropies from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2006, 8, 5385-5395.	2.8	69
45	The transition state for peptide bond formation reveals the ribosome as a water trap. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1888-1893.	7.1	69
46	Computational Prediction of Structure, Substrate Binding Mode, Mechanism, and Rate for a Malaria Protease with a Novel Type of Active Site. Biochemistry, 2004, 43, 14521-14528.	2.5	68
47	Toward a Consensus Model of the hERG Potassium Channel. ChemMedChem, 2010, 5, 455-467.	3.2	66
48	Principles of stop-codon reading on the ribosome. Nature, 2010, 465, 947-950.	27.8	64
49	Analysis of Electrostatic Potential Truncation Schemes in Simulations of Polar Solvents. Journal of Physical Chemistry B, 1998, 102, 3837-3840.	2.6	63
50	Protein Surface Softness Is the Origin of Enzyme Cold-Adaptation of Trypsin. PLoS Computational Biology, 2014, 10, e1003813.	3.2	63
51	On the Reactivity of Phosphate Monoester Dianions in Aqueous Solution:Â BrÃ¸nsted Linear Free-Energy Relationships Do Not Have an Unique Mechanistic Interpretation. Journal of the American Chemical Society, 1998, 120, 11524-11525.	13.7	62
52	Computational and NMR study of quaternary ammonium ion conformations in solution. Physical Chemistry Chemical Physics, 2002, 4, 4640-4647.	2.8	62
53	Synthesis of Malarial Plasmepsin Inhibitors and Prediction of Binding Modes by Molecular Dynamics Simulations. Journal of Medicinal Chemistry, 2005, 48, 6090-6106.	6.4	61
54	Ligand Binding to the Voltage-Gated Kv1.5 Potassium Channel in the Open Stateâ€”Docking and Computer Simulations of a Homology Model. Biophysical Journal, 2008, 94, 820-831.	0.5	60

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55	Probing the Effect of Point Mutations at Protein-Protein Interfaces with Free Energy Calculations. Biophysical Journal, 2006, 90, 433-442.	0.5	59
56	Computational Prediction of Alanine Scanning and Ligand Binding Energetics in G-Protein Coupled Receptors. PLoS Computational Biology, 2014, 10, e1003585.	3.2	58
57	Computation of affinity and selectivity: binding of 2,4-diaminopteridine and 2,4-diaminoquinazoline inhibitors to dihydrofolate reductases. Journal of Computer-Aided Molecular Design, 1998, 12, 119-131.	2.9	56
58	Computational Study of the Binding Affinity and Selectivity of the Bacterial Ammonium Transporter AmtBâ€. Biochemistry, 2006, 45, 10807-10814.	2.5	56
59	Protein Autoproteolysis: Conformational Strain Linked to the Rate of Peptide Cleavage by the pH Dependence of the N â†' O Acyl Shift Reaction. Journal of the American Chemical Society, 2009, 131, 9475-9477.	13.7	56
60	Continuum Solvation Models in the Linear Interaction Energy Method. Journal of Physical Chemistry B, 2006, 110, 12034-12041.	2.6	52
61	QligFEP: an automated workflow for small molecule free energy calculations in Q. Journal of Cheminformatics, 2019, 11, 26.	6.1	51
62	Structure-Based Energetics of mRNA Decoding on the Ribosome. Biochemistry, 2014, 53, 1714-1722.	2.5	50
63	Enzyme catalysis by entropy without Circe effect. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 2406-2411.	7.1	50
64	Computational modeling of enzymatic keto-enol isomerization reactions. Theoretical Chemistry Accounts, 2002, 108, 71-84.	1.4	49
65	Computer Simulation of Primary Kinetic Isotope Effects in the Proposed Rate-limiting Step of the Glyoxalase I Catalyzed Reaction. Journal of Biological Chemistry, 2000, 275, 22657-22662.	3.4	48
66	The Deacylation Step of Acetylcholinesterase:Â Computer Simulation Studies. Journal of the American Chemical Society, 2000, 122, 12254-12262.	13.7	48
67	The Catalytic Power of Ketosteroid Isomerase Investigated by Computer Simulationâ€. Biochemistry, 2002, 41, 15728-15735.	2.5	48
68	Modeling the mechanisms of biological GTP hydrolysis. Archives of Biochemistry and Biophysics, 2015, 582, 80-90.	3.0	48
69	Computational analysis of binding of P1 variants to trypsin. Protein Science, 2001, 10, 1584-1595.	7.6	47
70	Energetics of activation of GTP hydrolysis on the ribosome. Nature Communications, 2013, 4, 1733.	12.8	47
71	Chemical reaction mechanisms in solution from brute force computational Arrhenius plots. Nature Communications, 2015, 6, 7293.	12.8	47
72	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. SoftwareX, 2018, 7, 388-395.	2.6	47

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73	C2-Symmetric inhibitors of Plasmodium falciparum plasmepsin II: synthesis and theoretical predictions. Bioorganic and Medicinal Chemistry, 2003, 11, 3723-3733.	3.0	46
74	The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. Journal of the American Chemical Society, 2016, 138, 10664-10673.	13.7	46
75	Structural and Energetic Effects of A2A Adenosine Receptor Mutations on Agonist and Antagonist Binding. PLoS ONE, 2014, 9, e108492.	2.5	46
76	Computational modelling of inhibitor binding to human thrombin. European Journal of Pharmaceutical Sciences, 2001, 12, 441-446.	4.0	45
77	Computational inhibitor design against malaria plasmepsins. Cellular and Molecular Life Sciences, 2007, 64, 2285-2305.	5.4	43
78	A simple way to calculate the axis of an Î±-helix. Computers & Chemistry, 1986, 10, 97-99.	1.2	41
79	Absolute Hydration Entropies of Alkali Metal Ions from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 10255-10260.	2.6	41
80	Codon-reading specificities of mitochondrial release factors and translation termination at non-standard stop codons. Nature Communications, 2013, 4, 2940.	12.8	41
81	Modelling of ion-ligand interactions in solutions and biomolecules. Computational and Theoretical Chemistry, 1992, 256, 135-152.	1.5	40
82	Macrocyclic inhibitors of the malarial aspartic proteases plasmepsin I, II, and IV. Bioorganic and Medicinal Chemistry, 2006, 14, 2197-2208.	3.0	39
83	Role of Ribosomal Protein L27 in Peptidyl Transfer. Biochemistry, 2008, 47, 4898-4906.	2.5	39
84	Electrostatic effects play a central role in cold adaptation of trypsin. FEBS Letters, 2001, 499, 171-175.	2.8	38
85	Mechanism of the Translation Termination Reaction on the Ribosome. Biochemistry, 2009, 48, 11296-11303.	2.5	38
86	Computer Simulations of Structureâ€“Activity Relationships for hERG Channel Blockers. Biochemistry, 2011, 50, 6146-6156.	2.5	38
87	Comment on â€œThe Mechanism for Activation of GTP Hydrolysis on the Ribosomeâ€• Science, 2011, 333, 37-37.	12.6	38
88	Computational Predictions of Binding Affinities to Dihydrofolate Reductase:â€‰ Synthesis and Biological Evaluation of Methotrexate Analogues. Journal of Medicinal Chemistry, 2000, 43, 3852-3861.	6.4	36
89	Î±-Substituted norstatines as the transition-state mimic in inhibitors of multiple digestive vacuole malaria aspartic proteases. Bioorganic and Medicinal Chemistry, 2009, 17, 5933-5949.	3.0	36
90	Binding to and Inhibition of Insulin-Regulated Aminopeptidase by Macrocyclic Disulfides Enhances Spine Density. Molecular Pharmacology, 2016, 89, 413-424.	2.3	35

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91	Computer simulations explain the anomalous temperature optimum in a cold-adapted enzyme. Nature Communications, 2020, 11, 2644.	12.8	35
92	Predicting Binding Modes from Free Energy Calculations. Journal of Medicinal Chemistry, 2008, 51, 2657-2667.	6.4	34
93	Free energy calculations of A_{2A}adenosine receptor mutation effects on agonist binding. Chemical Communications, 2015, 51, 3522-3525.	4.1	33
94	Principles of start codon recognition in eukaryotic translation initiation. Nucleic Acids Research, 2016, 44, 8425-8432.	14.5	33
95	QresFEP: An Automated Protocol for Free Energy Calculations of Protein Mutations in Q. Journal of Chemical Theory and Computation, 2019, 15, 5461-5473.	5.3	33
96	Computer Simulation of Phenyl Ester Cleavage by Î²-Cyclodextrin in Solution. Journal of the American Chemical Society, 1998, 120, 6131-6137.	13.7	32
97	Exceptionally large entropy contributions enable the high rates of GTP hydrolysis on the ribosome. Scientific Reports, 2015, 5, 15817.	3.3	31
98	Permeation Redux: Thermodynamics and Kinetics of Ion Movement through Potassium Channels. Biophysical Journal, 2014, 106, 1859-1863.	0.5	30
99	The Conformation of a Catalytic Loop Is Central to GTPase Activity on the Ribosome. Biochemistry, 2015, 54, 546-556.	2.5	30
100	Structure-Based Design of Potent and Selective Ligands at the Four Adenosine Receptors. Molecules, 2017, 22, 1945.	3.8	30
101	Computational modelling of the open-state Kv1.5 ion channel block by bupivacaine. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2003, 1652, 35-51.	2.3	29
102	Energetics of Codonâ˜'Anticodon Recognition on the Small Ribosomal Subunitâ€. Biochemistry, 2007, 46, 200-209.	2.5	29
103	Inhibitor Binding to the Plasmepsin IV Aspartic Protease from Plasmodium falciparum. Biochemistry, 2006, 45, 10529-10541.	2.5	28
104	Elucidation of the Binding Mode of the Carboxyterminal Region of Peptide YY to the Human Y₂Receptor. Molecular Pharmacology, 2018, 93, 323-334.	2.3	28
105	Why base tautomerization does not cause errors in mRNA decoding on the ribosome. Nucleic Acids Research, 2014, 42, 12876-12884.	14.5	27
106	Aryl Sulfonamide Inhibitors of Insulin-Regulated Aminopeptidase Enhance Spine Density in Primary Hippocampal Neuron Cultures. ACS Chemical Neuroscience, 2016, 7, 1383-1392.	3.5	27
107	Energetics of the proposed rate-determining step of the glyoxalase I reaction. FEBS Letters, 1999, 453, 90-94.	2.8	25
108	The GPR139 reference agonists 1a and 7c, and tryptophan and phenylalanine share a common binding site. Scientific Reports, 2017, 7, 1128.	3.3	25

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109	Bridging the gap between ribosome structure and biochemistry by mechanistic computations. Current Opinion in Structural Biology, 2012, 22, 815-823.	5.7	24
110	Conserved Motifs in Different Classes of GTPases Dictate their Specific Modes of Catalysis. ACS Catalysis, 2016, 6, 1737-1743.	11.2	24
111	Cold Adaptation of Triosephosphate Isomerase. Biochemistry, 2017, 56, 4169-4176.	2.5	24
112	Computational modeling of the rate limiting step in low molecular weight protein tyrosine phosphatase. FEBS Letters, 1999, 456, 301-305.	2.8	23
113	Structure-activity relationship for extracellular block of K+ channels by tetraalkylammonium ions. FEBS Letters, 2003, 554, 159-164.	2.8	23
114	Mutagenesis and Computational Modeling of Human G-Protein-Coupled Receptor Y2 for Neuropeptide Y and Peptide YY. Biochemistry, 2013, 52, 7987-7998.	2.5	23
115	Xâ€Ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A_{2A} Adenosine Receptor Antagonists. Angewandte Chemie - International Edition, 2020, 59, 16536-16543.	13.8	23
116	Free-energy perturbation calculations of binding and transition-state energies: hydrolysis of phenyl esters by Î²-cyclodextrin. Chemical Physics Letters, 1999, 302, 267-272.	2.6	22
117	Mechanism of substrate dephosphorylation in lowMr protein tyrosine phosphatase. , 1999, 36, 370-379.		22
118	Design, synthesis, and computational affinity prediction of ester soft drugs as inhibitors of dihydrofolate reductase from Pneumocystis carinii. European Journal of Pharmaceutical Sciences, 2004, 22, 43-54.	4.0	22
119	Computational analysis of plasmepsin IV bound to an allophenylnorstatine inhibitor. FEBS Letters, 2006, 580, 5910-5916.	2.8	21
120	Complementary charge-based interaction between the ribosomal-stalk protein L7/12 and IF2 is the key to rapid subunit association. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 4649-4654.	7.1	21
121	A Role for the 2â€² OH of Peptidyl-tRNA Substrate in Peptide Release on the Ribosome Revealed through RF-Mediated Rescue. Chemistry and Biology, 2012, 19, 983-993.	6.0	20
122	Computational prediction of monosaccharide binding free energies to lectins with linear interaction energy models. Journal of Computational Chemistry, 2012, 33, 2340-2350.	3.3	20
123	Toward an Optimal Docking and Free Energy Calculation Scheme in Ligand Design with Application to COX-1 Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 1488-1499.	5.4	20
124	Binding Site Preorganization and Ligand Discrimination in the Purine Riboswitch. Journal of Physical Chemistry B, 2015, 119, 773-782.	2.6	20
125	Towards Rational Computational Engineering of Psychrophilic Enzymes. Scientific Reports, 2019, 9, 19147.	3.3	20
126	Molecular dynamics simulation of the solution structure of the C-terminal fragment of L7/L12 ribosomal protein. Biopolymers, 1990, 30, 205-209.	2.4	19

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127	Active Site of Epoxide Hydrolases Revisited:â€‰ A Noncanonical Residue in Potato StEH1 Promotes both Formation and Breakdown of the Alkylenzyme Intermediate. Biochemistry, 2007, 46, 2466-2479.	2.5	19
128	Molecular Mechanisms in the Selectivity of Nonsteroidal Anti-Inflammatory Drugs. Biochemistry, 2018, 57, 1236-1248.	2.5	19
129	3,4-Dihydropyrimidin-2(1H)-ones as Antagonists of the Human A_{2B} Adenosine Receptor: Optimization, Structureâ€“Activity Relationship Studies, and Enantiospecific Recognition. Journal of Medicinal Chemistry, 2021, 64, 458-480.	6.4	19
130	Catalytic Adaptation of Psychrophilic Elastase. Biochemistry, 2018, 57, 2984-2993.	2.5	18
131	Free energy calculations show that acidic P1 variants undergo large pKa shifts upon binding to trypsin. Proteins: Structure, Function and Bioinformatics, 2006, 64, 740-748.	2.6	17
132	Origin of the Enigmatic Stepwise Tight-Binding Inhibition of Cyclooxygenase-1. Biochemistry, 2015, 54, 7283-7291.	2.5	17
133	Energetic Tuning by tRNA Modifications Ensures Correct Decoding of Isoleucine and Methionine on the Ribosome. Chemistry - A European Journal, 2014, 20, 10271-10275.	3.3	16
134	Hidden Conformational States and Strange Temperature Optima in Enzyme Catalysis. Biochemistry, 2020, 59, 3844-3855.	2.5	16
135	A molecular model for the retinol binding protein-transthyretin complex. Journal of Molecular Graphics, 1992, 10, 120-123.	1.1	15
136	Long-range electrostatic effects on peptide folding. FEBS Letters, 1999, 457, 414-418.	2.8	15
137	Computational Study of the Influence of Solvent on16O/18O Equilibrium Isotope Effects in Phosphate Deprotonation Reactions. Journal of the American Chemical Society, 2002, 124, 10130-10135.	13.7	15
138	Peptide Release on the Ribosome Involves Substrate-Assisted Base Catalysis. ACS Catalysis, 2016, 6, 8432-8439.	11.2	15
139	Structural determinants of subtype selectivity and functional activity of angiotensin II receptors. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1355-1359.	2.2	15
140	Origin of the omnipotence of eukaryotic release factor 1. Nature Communications, 2017, 8, 1425.	12.8	15
141	Structure and mechanism of a phage-encoded SAM lyase revises catalytic function of enzyme family. ELife, 2021, 10, .	6.0	15
142	Computational Prediction of Structureâ^'Activity Relationships for the Binding of Aminocyclitols to Î²-Glucocerebrosidase. Journal of Chemical Information and Modeling, 2011, 51, 601-611.	5.4	14
143	Qgui: A high-throughput interface for automated setup and analysis of free energy calculations and empirical valence bond simulations in biological systems. Journal of Molecular Graphics and Modelling, 2015, 60, 15-23.	2.4	14
144	Effect of Nitrogen Atom Substitution in A₃ Adenosine Receptor Binding: N-(4,6-Diarylpyridin-2-yl)acetamides as Potent and Selective Antagonists. Journal of Medicinal Chemistry, 2017, 60, 7502-7511.	6.4	14

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145	Structural Basis of Inhibition of Human Insulin-Regulated Aminopeptidase (IRAP) by Aryl Sulfonamides. ACS Omega, 2018, 3, 4509-4521.	3.5	14
146	Sensitivity of an empirical affinity scoring function to changes in receptorâ€“ligand complex conformations. European Journal of Pharmaceutical Sciences, 2001, 14, 87-95.	4.0	13
147	Phe369(7.38) at human 5â€HT₇ receptors confers interspecies selectivity to antagonists and partial agonists. British Journal of Pharmacology, 2010, 159, 1069-1081.	5.4	13
148	Free energies underlying ion binding and transport in protein channels: free energy perturbation simulations of ion binding and selectivity for valinomycin. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 2099.	1.7	12
149	Computational modeling of catalysis and binding in low-molecular-weight protein tyrosine phosphatase. International Journal of Quantum Chemistry, 1999, 73, 147-159.	2.0	12
150	Charges for Large Scale Binding Free Energy Calculations with the Linear Interaction Energy Method. Journal of Chemical Theory and Computation, 2009, 5, 380-395.	5.3	12
151	Folding-Reaction Coupling in a Self-Cleaving Protein. Journal of Chemical Theory and Computation, 2012, 8, 3871-3879.	5.3	12
152	Evaluation of Adamantane Derivatives as Inhibitors of Dengue Virus mRNA Cap Methyltransferase by Docking and Molecular Dynamics Simulations. Molecular Informatics, 2013, 32, 155-164.	2.5	12
153	Mechanistic alternatives for peptide bond formation on the ribosome. Nucleic Acids Research, 2018, 46, 5345-5354.	14.5	12
154	Evolution of Angiotensin Peptides and Peptidomimetics as Angiotensin II Receptor Type 2 (AT2) Receptor Agonists. Biomolecules, 2020, 10, 649.	4.0	12
155	Computer Simulations Reveal Substrate Specificity of Glycosidic Bond Cleavage in Native and Mutant Human Purine Nucleoside Phosphorylase. Biochemistry, 2016, 55, 2153-2162.	2.5	11
156	Free Energy Calculations for Proteinâ€“Ligand Binding Prediction. Methods in Molecular Biology, 2021, 2266, 203-226.	0.9	11
157	Prediction of a ligand-induced conformational change in the catalytic core of Cdc25A. FEBS Letters, 2000, 465, 8-11.	2.8	10
158	Comparative Analysis of Putative Agonist-Binding Modes in the Human A1 Adenosine Receptor. ChemBioChem, 2004, 5, 841-849.	2.6	10
159	Computer-Aided Design of GPCR Ligands. Methods in Molecular Biology, 2015, 1272, 271-291.	0.9	10
160	Computer Simulations Reveal an Entirely Entropic Activation Barrier for the Chemical Step in a Designer Enzyme. ACS Catalysis, 2022, 12, 1452-1460.	11.2	10
161	Macrocyclic peptidomimetics as inhibitors of insulin-regulated aminopeptidase (IRAP). RSC Medicinal Chemistry, 2020, 11, 234-244.	3.9	9
162	Mutagenesis and Homology Modeling of the Tn21 Integron Integrase IntI1. Biochemistry, 2009, 48, 1743-1753.	2.5	8

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163	A close-up view of codon selection in eukaryotic initiation. RNA Biology, 2017, 14, 815-819.	3.1	8
164	A Series of Analogues to the AT₂R Prototype Antagonist C38 Allow Fine Tuning of the Previously Reported Antagonist Binding Mode. ChemistryOpen, 2019, 8, 114-125.	1.9	8
165	Dissecting the Mechanism of (R)-3-Hydroxybutyrate Dehydrogenase by Kinetic Isotope Effects, Protein Crystallography, and Computational Chemistry. ACS Catalysis, 2020, 10, 15019-15032.	11.2	8
166	Structure and Mechanism of a Cold-Adapted Bacterial Lipase. Biochemistry, 2022, 61, 933-942.	2.5	8
167	Principles of tRNA^{Ala} Selection by Alanylâ€“tRNA Synthetase Based on the Critical G3Â·U70 Base Pair. ACS Omega, 2019, 4, 15539-15548.	3.5	7
168	Free energy calculations of RNA interactions. Methods, 2019, 162-163, 85-95.	3.8	7
169	Synthesis, Evaluation and Proposed Binding Pose of Substituted Spiroâ€Oxindole Dihydroquinazolinones as IRAP Inhibitors. ChemistryOpen, 2020, 9, 325-337.	1.9	7
170	Characterization of Ligand Binding to GPCRs Through Computational Methods. Methods in Molecular Biology, 2018, 1705, 23-44.	0.9	6
171	Inhibition of translation termination by small molecules targeting ribosomal release factors. Scientific Reports, 2019, 9, 15424.	3.3	6
172	The Activation Parameters of a Cold-Adapted Short Chain Dehydrogenase Are Insensitive to Enzyme Oligomerization. Biochemistry, 2022, 61, 514-522.	2.5	6
173	Molecular dynamics study of heparin based coatings. Biomaterials, 2008, 29, 4463-4469.	11.4	5
174	Does Glutamine Methylation Affect the Intrinsic Conformation of the Universally Conserved GGQ Motif in Ribosomal Release Factors?. Biochemistry, 2009, 48, 3483-3489.	2.5	5
175	Probing the Time Dependency of Cyclooxygenase-1 Inhibitors by Computer Simulations. Biochemistry, 2017, 56, 1911-1920.	2.5	5
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