Amedeo Caflisch

List of Publications by Year
in descending order

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167	15,632	34493	21239
papers	citations	54 h-index	119 g-index

175	175	175	19427
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Thermostable designed ankyrin repeat proteins (DARPins) as building blocks for innovative drugs. Journal of Biological Chemistry, 2022, 298, 101403.	1.6	17
2	The role of the N-terminal amphipathic helix in bacterial YidC: Insights from functional studies, the crystal structure and molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183825.	1.4	10
3	Dynamics of the Histone Acetyltransferase Lysine-Rich Loop in the Catalytic Core of the CREB-Binding Protein. Journal of Chemical Information and Modeling, 2022, , .	2.5	3
4	Silybins inhibit human IAPP amyloid growth and toxicity through stereospecific interactions. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2022, 1870, 140772.	1.1	10
5	Structure-based design of ligands of the m6A-RNA reader YTHDC1. European Journal of Medicinal Chemistry Reports, 2022, 5, 100057.	0.6	3
6	Antibody binding modulates the dynamics ofÂtheÂmembrane-bound prion protein. Biophysical Journal, 2022, 121, 2813-2825.	0.2	3
7	Flanking sequence preference modulates de novo DNA methylation in the mouse genome. Nucleic Acids Research, 2021, 49, 145-157.	6.5	14
8	Dynamic 3D proteomes reveal protein functional alterations at high resolution in situ. Cell, 2021, 184, 545-559.e22.	13.5	82
9	Atomistic and Thermodynamic Analysis of N6-Methyladenosine (m⁶A) Recognition by the Reader Domain of YTHDC1. Journal of Chemical Theory and Computation, 2021, 17, 1240-1249.	2.3	18
10	Proteostasis of Islet Amyloid Polypeptide: A Molecular Perspective of Risk Factors and Protective Strategies for Type II Diabetes. Chemical Reviews, 2021, 121, 1845-1893.	23.0	129
11	Combined computational and cellular screening identifies synergistic inhibition of SARS-CoV-2 by lenvatinib and remdesivir. Journal of General Virology, 2021, 102, .	1.3	4
12	METTL3 Inhibitors for Epitranscriptomic Modulation of Cellular Processes. ChemMedChem, 2021, 16, 3035-3043.	1.6	87
13	Identification of a BAZ2A Bromodomain Hit Compound by Fragment Joining. ACS Bio & Med Chem Au, 2021, 1, 5-10.	1.7	3
14	Enhancer RNA m6A methylation facilitates transcriptional condensate formation and gene activation. Molecular Cell, 2021, 81, 3368-3385.e9.	4.5	135
15	1,4,9-Triazaspiro[5.5]undecan-2-one Derivatives as Potent and Selective METTL3 Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 12738-12760.	2.9	55
16	Unsupervised Methods for Detection of Neural States: Case Study of Hippocampal-Amygdala Interactions. ENeuro, 2021, 8, ENEURO.0484-20.2021.	0.9	2
17	The 3A6â€TCR/superagonist/HLAâ€ÐR2a complex shows similar interface and reduced flexibility compared to the complex with selfâ€peptide. Proteins: Structure, Function and Bioinformatics, 2020, 88, 31-46.	1.5	0
18	Structural and Dynamic Insights into Redundant Function of YTHDF Proteins. Journal of Chemical Information and Modeling, 2020, 60, 5932-5935.	2.5	37

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19	An ABSINTH-Based Protocol for Predicting Binding Affinities between Proteins and Small Molecules. Journal of Chemical Information and Modeling, 2020, 60, 5188-5202.	2.5	5
20	Assessment of the Fragment Docking Program SEED. Journal of Chemical Information and Modeling, 2020, 60, 4881-4893.	2.5	9
21	<scp>Sapphire</scp>-Based Clustering. Journal of Chemical Theory and Computation, 2020, 16, 6383-6396.	2.3	13
22	Smallâ€Molecule Inhibitors of METTL3, the Major Human Epitranscriptomic Writer. ChemMedChem, 2020, 15, 744-748.	1.6	106
23	Hitting a Moving Target: Simulation and Crystallography Study of ATAD2 Bromodomain Blockers. ACS Medicinal Chemistry Letters, 2020, 11, 1573-1580.	1.3	8
24	Selectively Disrupting m⁶A-Dependent Proteinâ€“RNA Interactions with Fragments. ACS Chemical Biology, 2020, 15, 618-625.	1.6	17
25	Kinetic Control of Amyloidogenesis Calls for Unconventional Drugs To Fight Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2020, 11, 103-104.	1.7	6
26	Synthesis, radiolabelling and initial biological characterisation of 18F-labelled xanthine derivatives for PET imaging of Eph receptors. Organic and Biomolecular Chemistry, 2020, 18, 3104-3116.	1.5	8
27	Understanding the mechanism of action of pyrrolo[3,2-b]quinoxaline-derivatives as kinase inhibitors. RSC Medicinal Chemistry, 2020, 11, 665-675.	1.7	4
28	Flexible Binding of m⁶A Reader Protein YTHDC1 to Its Preferred RNA Motif. Journal of Chemical Theory and Computation, 2019, 15, 7004-7014.	2.3	18
29	A Reader-Based Assay for m⁶A Writers and Erasers. Analytical Chemistry, 2019, 91, 3078-3084.	3.2	36
30	Ligand retargeting by binding site analogy. European Journal of Medicinal Chemistry, 2019, 175, 107-113.	2.6	2
31	On the removal of initial state bias from simulation data. Journal of Chemical Physics, 2019, 150, 104105.	1.2	12
32	Simulation Studies of Amyloidogenic Polypeptides and Their Aggregates. Chemical Reviews, 2019, 119, 6956-6993.	23.0	138
33	Unsupervised identification of states from voltage recordings of neural networks. Journal of Neuroscience Methods, 2019, 318, 104-117.	1.3	3
34	Cover Image, Volume 87, Issue 2. Proteins: Structure, Function and Bioinformatics, 2019, 87, C4.	1.5	0
35	Disulfide bridge formation influences ligand recognition by the ATAD2 bromodomain. Proteins: Structure, Function and Bioinformatics, 2019, 87, 157-167.	1.5	9
36	Editorial overview: Folding and binding: In silico, in vitro and in cellula. Current Opinion in Structural Biology, 2018, 48, iv-vii.	2.6	0

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37	Chemical Space Expansion of Bromodomain Ligands Guided by in Silico Virtual Couplings (AutoCouple). ACS Central Science, 2018, 4, 180-188.	5.3	26
38	Iriomoteolides: novel chemical tools to study actin dynamics. Chemical Science, 2018, 9, 3793-3802.	3.7	8
39	Protein structure-based drug design: from docking to molecular dynamics. Current Opinion in Structural Biology, 2018, 48, 93-102.	2.6	405
40	In Silico Identification of JMJD3 Demethylase Inhibitors. Journal of Chemical Information and Modeling, 2018, 58, 2151-2163.	2.5	10
41	Structural Analysis of Smallâ€Molecule Binding to the BAZ2A and BAZ2B Bromodomains. ChemMedChem, 2018, 13, 1479-1487.	1.6	11
42	Structure-based discovery of selective BRPF1 bromodomain inhibitors. European Journal of Medicinal Chemistry, 2018, 155, 337-352.	2.6	26
43	Disorder at the Tips of a Disease-Relevant AÎ²42 Amyloid Fibril: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 11072-11082.	1.2	24
44	Serotonin uptake is required for Rac1 activation in Krasâ€induced acinarâ€toâ€ductal metaplasia in the pancreas. Journal of Pathology, 2018, 246, 352-365.	2.1	13
45	In silico fragment-based drug design with SEED. European Journal of Medicinal Chemistry, 2018, 156, 907-917.	2.6	18
46	Binding Motifs in the CBP Bromodomain: An Analysis of 20 Crystal Structures of Complexes with Small Molecules. ACS Medicinal Chemistry Letters, 2018, 9, 929-934.	1.3	8
47	Virtual screen to NMR (VS2NMR): Discovery of fragment hits for the CBP bromodomain. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2472-2478.	1.0	18
48	N,N Dimethylacetamide a drug excipient that acts as bromodomain ligand for osteoporosis treatment. Scientific Reports, 2017, 7, 42108.	1.6	22
49	Discovery of BAZ2A bromodomain ligands. European Journal of Medicinal Chemistry, 2017, 139, 564-572.	2.6	21
50	Discovery of Inhibitors of Four Bromodomains by Fragment-Anchored Ligand Docking. Journal of Chemical Information and Modeling, 2017, 57, 2584-2597.	2.5	21
51	Amyloid Î² Fibril Elongation by Monomers Involves Disorder at the Tip. Journal of Chemical Theory and Computation, 2017, 13, 5117-5130.	2.3	34
52	Reducing the Flexibility of Typeâ€…II Dehydroquinase for Inhibition: A Fragmentâ€Based Approach and Molecular Dynamics Study. ChemMedChem, 2017, 12, 1512-1524.	1.6	4
53	The ATAD2 bromodomain binds different acetylation marks on the histone H4 in similar fuzzy complexes. Journal of Biological Chemistry, 2017, 292, 16734-16745.	1.6	26
54	Proteomic analyses identify ARH3 as a serine mono-ADP-ribosylhydrolase. Nature Communications, 2017, 8, 2055.	5.8	98

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55	Focused conformational sampling in proteins. Journal of Chemical Physics, 2017, 147, 195102.	1.2	8
56	Specific Inhibition of Î²-Secretase Processing of the Alzheimer Disease Amyloid Precursor Protein. Cell Reports, 2016, 14, 2127-2141.	2.9	87
57	Twenty Crystal Structures of Bromodomain and PHD Finger Containing Protein 1 (BRPF1)/Ligand Complexes Reveal Conserved Binding Motifs and Rare Interactions. Journal of Medicinal Chemistry, 2016, 59, 5555-5561.	2.9	33
58	Derivatives of 3-Amino-2-methylpyridine as BAZ2B Bromodomain Ligands: In Silico Discovery and in Crystallo Validation. Journal of Medicinal Chemistry, 2016, 59, 9919-9927.	2.9	23
59	Computationally Designed Armadillo Repeat Proteins for Modular Peptide Recognition. Journal of Molecular Biology, 2016, 428, 4467-4489.	2.0	19
60	A Small-Molecule Inhibitor of Lin28. ACS Chemical Biology, 2016, 11, 2773-2781.	1.6	121
61	Fragment-based in silico screening of bromodomain ligands. Drug Discovery Today: Technologies, 2016, 19, 81-90.	4.0	12
62	Dynamic microfluidic control of supramolecular peptide self-assembly. Nature Communications, 2016, 7, 13190.	5.8	89
63	Data publication with the structural biology data grid supports live analysis. Nature Communications, 2016, 7, 10882.	5.8	113
64	Fragment-Based Design of Selective Nanomolar Ligands of the CREBBP Bromodomain. Journal of Medicinal Chemistry, 2016, 59, 1350-1356.	2.9	54
65	The â€œGatekeeperâ€•Residue Influences the Mode of Binding of Acetyl Indoles to Bromodomains. Journal of Medicinal Chemistry, 2016, 59, 3087-3097.	2.9	36
66	Protein Structural Memory Influences Ligand Binding Mode(s) and Unbinding Rates. Journal of Chemical Theory and Computation, 2016, 12, 1393-1399.	2.3	6
67	Three stories on Eph kinase inhibitors: From in silico discovery to inÂvivo validation. European Journal of Medicinal Chemistry, 2016, 112, 347-366.	2.6	24
68	High-Throughput Fragment Docking into the BAZ2B Bromodomain: Efficient in Silico Screening for X-Ray Crystallography. ACS Chemical Biology, 2016, 11, 800-807.	1.6	32
69	Discovery of CREBBP Bromodomain Inhibitors by High-Throughput Docking and Hit Optimization Guided by Molecular Dynamics. Journal of Medicinal Chemistry, 2016, 59, 1340-1349.	2.9	70
70	A Combined NMR and Computational Approach to Investigate Peptide Binding to a Designed Armadillo Repeat Protein. Journal of Molecular Biology, 2015, 427, 1916-1933.	2.0	6
71	The roles of the conserved tyrosine in the Î²2-Î±2 loop of the prion protein. Prion, 2015, 9, 412-419.	0.9	10
72	Evolutionary Conserved Tyr169 Stabilizes the Î²2-Î±2 Loop of the Prion Protein. Journal of the American Chemical Society, 2015, 137, 2948-2957.	6.6	36

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73	Structural Analysis of the Binding of Type I, I_{1/2}, and II Inhibitors to Eph Tyrosine Kinases. ACS Medicinal Chemistry Letters, 2015, 6, 79-83.	1.3	9
74	Binding Mode of Acetylated Histones to Bromodomains: Variations on a Common Motif. ChemMedChem, 2015, 10, 1327-1333.	1.6	28
75	Structure-based drug design identifies polythiophenes as antiprion compounds. Science Translational Medicine, 2015, 7, 299ra123.	5.8	130
76	Current kinase inhibitors cover a tiny fraction of fragment space. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2372-2376.	1.0	20
77	Peptide Binding to a PDZ Domain by Electrostatic Steering via Nonnative Salt Bridges. Biophysical Journal, 2015, 108, 2362-2370.	0.2	36
78	Weighted Distance Functions Improve Analysis of High-Dimensional Data: Application to Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 5481-5492.	2.3	11
79	Molecular dynamics in drug design. European Journal of Medicinal Chemistry, 2015, 91, 4-14.	2.6	174
80	A molecular simulation protocol to avoid sampling redundancy and discover new states. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 889-902.	1.1	25
81	Specificity and mechanism-of-action of the JAK2 tyrosine kinase inhibitors ruxolitinib and SAR302503 (TG101348). Leukemia, 2014, 28, 404-407.	3.3	98
82	Structured Water Molecules in the Binding Site of Bromodomains Can Be Displaced by Cosolvent. ChemMedChem, 2014, 9, 573-579.	1.6	44
83	A novel allosteric mechanism in the cysteine peptidase cathepsin K discovered by computational methods. Nature Communications, 2014, 5, 3287.	5.8	77
84	Discovery of dual ZAP70 and Syk kinases inhibitors by docking into a rare C-helix-out conformation of Syk. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 1523-1527.	1.0	27
85	Discovery of BRD4 bromodomain inhibitors by fragment-based high-throughput docking. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2493-2496.	1.0	61
86	Molecular Dynamics Simulations of Bromodomains Reveal Bindingâ€Site Flexibility and Multiple Binding Modes of the Natural Ligand Acetylâ€Lysine. Israel Journal of Chemistry, 2014, 54, 1084-1092.	1.0	22
87	Spontaneous Self-Assembly of Engineered Armadillo Repeat Protein Fragments into a Folded Structure. Structure, 2014, 22, 985-995.	1.6	19
88	Pyrrolo[3,2-b]quinoxaline Derivatives as Types I_{1/2} and II Eph Tyrosine Kinase Inhibitors: Structure-Based Design, Synthesis, and in Vivo Validation. Journal of Medicinal Chemistry, 2014, 57, 6834-6844.	2.9	27
89	Equilibrium Sampling Approach to the Interpretation of Electron Density Maps. Structure, 2014, 22, 156-167.	1.6	9
90	High-Resolution Visualisation of the States and Pathways Sampled in Molecular Dynamics Simulations. Scientific Reports, 2014, 4, 6264.	1.6	17

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91	Mechanism and Kinetics of Acetyl-Lysine Binding to Bromodomains. Journal of Chemical Theory and Computation, 2013, 9, 4225-4232.	2.3	26
92	Does bromodomain flexibility influence histone recognition?. FEBS Letters, 2013, 587, 2158-2163.	1.3	37
93	Optimization of Inhibitors of the Tyrosine Kinase EphB4. 2. Cellular Potency Improvement and Binding Mode Validation by X-ray Crystallography. Journal of Medicinal Chemistry, 2013, 56, 84-96.	2.9	26
94	A scalable algorithm to order and annotate continuous observations reveals the metastable states visited by dynamical systems. Computer Physics Communications, 2013, 184, 2446-2453.	3.0	24
95	Free Energy Guided Sampling. Journal of Chemical Theory and Computation, 2012, 8, 3423-3423.	2.3	2
96	Ultrametricity in Protein Folding Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 1580-1588.	2.3	2
97	How Does Darunavir Prevent HIV-1 Protease Dimerization?. Journal of Chemical Theory and Computation, 2012, 8, 1786-1794.	2.3	23
98	Efficient Construction of Mesostate Networks from Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2012, 8, 1108-1120.	2.3	42
99	50 Years of Lifsonâ€“Roig Models: Application to Molecular Simulation Data. Journal of Chemical Theory and Computation, 2012, 8, 363-373.	2.3	21
100	Free Energy Guided Sampling. Journal of Chemical Theory and Computation, 2012, 8, 2134-2140.	2.3	23
101	Optimization of designed armadillo repeat proteins by molecular dynamics simulations and NMR spectroscopy. Protein Science, 2012, 21, 1298-1314.	3.1	34
102	Distribution of Reciprocal of Interatomic Distances: A Fast Structural Metric. Journal of Chemical Theory and Computation, 2012, 8, 2930-2937.	2.3	45
103	Equilibrium Distribution from Distributed Computing (Simulations of Protein Folding). Journal of Physical Chemistry B, 2011, 115, 6358-6365.	1.2	17
104	In silicoidentification and crystal structure validation of caspase-3 inhibitors without a P1 aspartic acid moiety. Acta Crystallographica Section F: Structural Biology Communications, 2011, 67, 842-850.	0.7	14
105	Small Molecule Binding to Proteins: Affinity and Binding/Unbinding Dynamics from Atomistic Simulations. ChemMedChem, 2011, 6, 1578-1580.	1.6	33
106	Disordered Binding of Small Molecules to AÎ²(12â€“28). Journal of Biological Chemistry, 2011, 286, 41578-41588.	1.6	46
107	Library screening by fragmentâ€based docking. Journal of Molecular Recognition, 2010, 23, 183-193.	1.1	32
108	Highâ€Throughput Virtual Screening Using Quantum Mechanical Probes: Discovery of Selective Kinase Inhibitors. ChemMedChem, 2010, 5, 1007-1014.	1.6	35

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109	Amyloid Fibril Polymorphism Is under Kinetic Control. Journal of the American Chemical Society, 2010, 132, 14960-14970.	6.6	125
110	Crowding Effects on Amyloid Aggregation Kinetics. Journal of Physical Chemistry Letters, 2010, 1, 3027-3032.	2.1	50
111	Micelle-Like Architecture of the Monomer Ensemble of Alzheimerâ€™s Amyloid-Î² Peptide in Aqueous Solution and Its Implications for AÎ² Aggregation. Journal of Molecular Biology, 2010, 403, 148-165.	2.0	71
112	Discovery of a Non-Peptidic Inhibitor of West Nile Virus NS3 Protease by High-Throughput Docking. PLoS Neglected Tropical Diseases, 2009, 3, e356.	1.3	71
113	Discovery of Plasmepsin Inhibitors by Fragmentâ€Based Docking and Consensus Scoring. ChemMedChem, 2009, 4, 1317-1326.	1.6	49
114	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	1.5	7,077
115	Flaviviral Protease Inhibitors Identified by Fragment-Based Library Docking into a Structure Generated by Molecular Dynamics. Journal of Medicinal Chemistry, 2009, 52, 4860-4868.	2.9	77
116	Amyloid Aggregation on Lipid Bilayers and Its Impact on Membrane Permeability. Journal of Molecular Biology, 2009, 387, 407-415.	2.0	133
117	Structure-Based Optimization of Potent and Selective Inhibitors of the Tyrosine Kinase Erythropoietin Producing Human Hepatocellular Carcinoma Receptor B4 (EphB4). Journal of Medicinal Chemistry, 2009, 52, 6433-6446.	2.9	84
118	Structureâ€based tailoring of compound libraries for highâ€throughput screening: Discovery of novel EphB4 kinase inhibitors. Proteins: Structure, Function and Bioinformatics, 2008, 73, 11-18.	1.5	64
119	One-Dimensional Barrier-Preserving Free-Energy Projections of a Î²-sheet Miniprotein: New Insights into the Folding Process. Journal of Physical Chemistry B, 2008, 112, 8701-8714.	1.2	78
120	A doubleâ€headed cathepsin B inhibitor devoid of warhead. Protein Science, 2008, 17, 2145-2155.	3.1	36
121	Characterization and Further Stabilization of Designed Ankyrin Repeat Proteins by Combining Molecular Dynamics Simulations and Experiments. Journal of Molecular Biology, 2008, 375, 837-854.	2.0	77
122	Designed Armadillo Repeat Proteins as General Peptide-Binding Scaffolds: Consensus Design and Computational Optimization of the Hydrophobic Core. Journal of Molecular Biology, 2008, 376, 1282-1304.	2.0	108
123	Is Quantum Mechanics Necessary for Predicting Binding Free Energy?. Journal of Medicinal Chemistry, 2008, 51, 4280-4288.	2.9	53
124	Discovery of Kinase Inhibitors by High-Throughput Docking and Scoring Based on a Transferable Linear Interaction Energy Model. Journal of Medicinal Chemistry, 2008, 51, 1179-1188.	2.9	57
125	Fragment-Based de Novo Ligand Design by Multiobjective Evolutionary Optimization. Journal of Chemical Information and Modeling, 2008, 48, 679-690.	2.5	132
126	Pathways and Intermediates of Amyloid Fibril Formation. Journal of Molecular Biology, 2007, 374, 917-924.	2.0	132

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127	In Silico Discovery of Î²-Secretase Inhibitors. Journal of the American Chemical Society, 2006, 128, 5436-5443.	6.6	93
128	Automatic and Efficient Decomposition of Two-Dimensional Structures of Small Molecules for Fragment-Based High-Throughput Docking. Journal of Medicinal Chemistry, 2006, 49, 7384-7392.	2.9	87
129	A Molecular Dynamics Approach to the Structural Characterization of Amyloid Aggregation. Journal of Molecular Biology, 2006, 357, 1306-1321.	2.0	85
130	Interpreting the Aggregation Kinetics of Amyloid Peptides. Journal of Molecular Biology, 2006, 360, 882-892.	2.0	239
131	Computational models for the prediction of polypeptide aggregation propensity. Current Opinion in Chemical Biology, 2006, 10, 437-444.	2.8	124
132	Network and graph analyses of folding free energy surfaces. Current Opinion in Structural Biology, 2006, 16, 71-78.	2.6	72
133	Estimation of protein folding probability from equilibrium simulations. Journal of Chemical Physics, 2005, 122, 184901.	1.2	35
134	Discovery of Cell-Permeable Non-Peptide Inhibitors of Î²-Secretase by High-Throughput Docking and Continuum Electrostatics Calculations#. Journal of Medicinal Chemistry, 2005, 48, 5108-5111.	2.9	90
135	Protein Folding. Structure, 2004, 12, 1750-1752.	1.6	4
136	Automated docking of highly flexible ligands by genetic algorithms: A critical assessment. Journal of Computational Chemistry, 2004, 25, 412-422.	1.5	56
137	Efficient Evaluation of Binding Free Energy Using Continuum Electrostatics Solvation. Journal of Medicinal Chemistry, 2004, 47, 5791-5797.	2.9	103
138	Folding for binding or binding for folding?. Trends in Biotechnology, 2003, 21, 423-425.	4.9	19
139	The role of side-chain interactions in the early steps of aggregation: Molecular dynamics simulations of an amyloid-forming peptide from the yeast prion Sup35. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 5154-5159.	3.3	257
140	Combining task- and data parallelism to speed up protein folding on a desktop grid platform. , 2003, , .		7
141	Replica exchange molecular dynamics simulations of reversible folding. Journal of Chemical Physics, 2003, 119, 4035-4042.	1.2	94
142	Performance characterization of a molecular dynamics code on PC clusters: is there any easy parallelism in CHARMM?. , 2002, , .		9
143	Efficient electrostatic solvation model for protein-fragment docking. Proteins: Structure, Function and Bioinformatics, 2001, 42, 256-268.	1.5	93
144	Structure-based ligand design by a build-up approach and genetic algorithm search in conformational space. Journal of Computational Chemistry, 2001, 22, 1956-1970.	1.5	23

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145	Fragment-Based Flexible Ligand Docking by Evolutionary Optimization. Biological Chemistry, 2001, 382, 1365-1372.	1.2	60
146	Computer simulations of protein folding by targeted molecular dynamics. , 2000, 39, 252-260.		69
147	Design of dimerization inhibitors of HIV-1 aspartic proteinase: a computer-based combinatorial approach. Journal of Computer-Aided Molecular Design, 2000, 14, 161-179.	1.3	23
148	Hydrophobicity maps and docking of molecular fragments with solvation. Journal of Computer - Aided Molecular Design, 2000, 20, 145-169.	1.0	7
149	Free Energy Surface of the Helical Peptide Y(MEARA)6. Journal of Physical Chemistry B, 2000, 104, 10080-10086.	1.2	58
150	Targeted Molecular Dynamics Simulations of Protein Unfolding. Journal of Physical Chemistry B, 2000, 104, 4511-4518.	1.2	46
151	Thermodynamics and Kinetics of Folding of Two Model Peptides Investigated by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2000, 104, 5000-5010.	1.2	140
152	Calculation of conformational transitions and barriers in solvated systems: Application to the alanine dipeptide in water. Journal of Chemical Physics, 1999, 110, 2099-2108.	1.2	182
153	Comment on the validation of continuum electrostatics models. Journal of Computational Chemistry, 1999, 20, 1533-1536.	1.5	17
154	Exhaustive docking of molecular fragments with electrostatic solvation. Proteins: Structure, Function and Bioinformatics, 1999, 37, 88-105.	1.5	171
155	Hydrophobicity at the surface of proteins. , 1999, 37, 565-575.		38
156	Exhaustive docking of molecular fragments with electrostatic solvation. , 1999, 37, 88.		6
157	Exhaustive docking of molecular fragments with electrostatic solvation. Proteins: Structure, Function and Bioinformatics, 1999, 37, 88-105.	1.5	31
158	Docking small ligands in flexible binding sites. Journal of Computational Chemistry, 1998, 19, 21-37.	1.5	120
159	Comparison of a GB Solvation Model with Explicit Solvent Simulations:Â Potentials of Mean Force and Conformational Preferences of Alanine Dipeptide and 1,2-Dichloroethane. Journal of Physical Chemistry B, 1998, 102, 3637-3641.	1.2	63
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161	Continuum Electrostatic Energies of Macromolecules in Aqueous Solutions. Journal of Physical Chemistry A, 1997, 101, 8098-8106.	1.1	131
162	Docking by Monte Carlo minimization with a solvation correction: Application to an FKBP?substrate complex. Journal of Computational Chemistry, 1997, 18, 723-743.	1.5	51

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163	Protein dynamics: From the native to the unfolded state and back again. Molecular Engineering, 1995, 5, 55-70.	0.2	1
164	Acid and Thermal Denaturation of Barnase Investigated by Molecular Dynamics Simulations. Journal of Molecular Biology, 1995, 252, 672-708.	2.0	171
165	Molecular dynamics simulation of protein denaturation: solvation of the hydrophobic cores and secondary structure of barnase.. Proceedings of the National Academy of Sciences of the United States of America, 1994, 91, 1746-1750.	3.3	164
166	Multiple copy simultaneous search and construction of ligands in binding sites: application to inhibitors of HIV-1 aspartic proteinase. Journal of Medicinal Chemistry, 1993, 36, 2142-2167.	2.9	209
167	Docking small ligands in flexible binding sites. , 0, .		1