Junmei Wang

List of Publications by Year in Descending Order

143 papers	30,310 citations	51 h-index	158 g-index
158 ext. papers	35,248 ext. citations	6.9 avg, IF	7.35 L-index

#	Paper	IF	Citations
143	In Silico Prediction of Pharmacokinetic Profile for Human Oral Drug Candidates Which Lack Clinical Pharmacokinetic Experiment Data.. *European Journal of Drug Metabolism and Pharmacokinetics*, **2022**, 1	2.7	1
142	RNPS1 inhibits excessive tumor necrosis factor/tumor necrosis factor receptor signaling to support hematopoiesis in mice.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2200128119	11.5	
141	Physiologically-Based Pharmacokinetics Modeling for Hydroxychloroquine as a Treatment for Malaria and Optimized Dosing Regimens for Different Populations. *Journal of Personalized Medicine* , **2022**, 12, 796	3.6	0
140	Recent progress in general force fields of small molecules.. *Current Opinion in Structural Biology*, **2021**, 72, 187-193	8.1	0
139	Machine learning on ligand-residue interaction profiles to significantly improve binding affinity prediction. *Briefings in Bioinformatics*, **2021**, 22,	13.4	4
138	VAD-MM/GBSA: A Variable Atomic Dielectric MM/GBSA Model for Improved Accuracy in Protein-Ligand Binding Free Energy Calculations. *Journal of Chemical Information and Modeling*, **2021**, 61, 2844-2856	6.1	2
137	In silico binding profile characterization of SARS-CoV-2 spike protein and its mutants bound to human ACE2 receptor. *Briefings in Bioinformatics*, **2021**, 22,	13.4	6
136	Drug-Drug Interaction Between Oxycodone and Diazepam by a Combined Pharmacokinetic and Pharmacodynamic Modeling Approach. *ACS Chemical Neuroscience*, **2021**, 12, 1777-1790	5.7	2
135	Molecular Mechanism of Ultrasound-Induced Structural Defects in Liposomes: A Nonequilibrium Molecular Dynamics Simulation Study. *Langmuir*, **2021**, 37, 7945-7954	4	1
134	Structure and dynamics of major histocompatibility class Ib molecule H2-M3 complexed with mitochondrial-derived peptides. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-13	3.6	
133	Sulfatides are endogenous ligands for the TLR4-MD-2 complex. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	4
132	Landscape of drug-resistance mutations in kinase regulatory hotspots. *Briefings in Bioinformatics*, **2021**, 22,	13.4	7
131	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. *Journal of Chemical Theory and Computation*, **2021**, 17, 1086-1097	6.4	5
130	Nonequilibrium molecular dynamics simulations of infrared laser-induced dissociation of a tetrameric A□2 □barrel in a neuronal membrane model. *Chemistry and Physics of Lipids*, **2021**, 234, 105030	3.7	2
129	Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. *Journal of Cheminformatics*, **2021**, 13, 11	8.6	0
128	Aicardi-Gouti□es syndrome-associated mutation at ADAR1 gene locus activates innate immune response in mouse brain. *Journal of Neuroinflammation*, **2021**, 18, 169	10.1	0
127	TMEM120A is a coenzyme A-binding membrane protein with structural similarities to ELOVL fatty acid elongase. *ELife*, **2021**, 10,	8.9	6

126	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of PHF6 Peptide of Tau Protein. *Journal of Chemical Theory and Computation*, **2021**, 17, 6458-6471	6.4	6
125	Orientation and dynamics of Cu based DNA labels from force field parameterized MD elucidates the relationship between EPR distance constraints and DNA backbone distances. *Physical Chemistry Chemical Physics*, **2020**, 22, 26707-26719	3.6	5
124	Infrared Laser-Induced Amyloid Fibril Dissociation: A Joint Experimental/Theoretical Study on the GNNQQNY Peptide. *Journal of Physical Chemistry B*, **2020**, 124, 6266-6277	3.4	10
123	Development and Evaluation of MM/GBSA Based on a Variable Dielectric GB Model for Predicting Protein-Ligand Binding Affinities. *Journal of Chemical Information and Modeling*, **2020**, 60, 5353-5365	6.1	13
122	Molecular Dynamics Simulations Based on Newly Developed Force Field Parameters for Cu Spin Labels Provide Insights into Double-Histidine-Based Double Electron-Electron Resonance. *Journal of Physical Chemistry B*, **2020**, 124, 2788-2797	3.4	15
121	Prediction of the Binding Affinities and Selectivity for CB1 and CB2 Ligands Using Homology Modeling, Molecular Docking, Molecular Dynamics Simulations, and MM-PBSA Binding Free Energy Calculations. *ACS Chemical Neuroscience*, **2020**, 11, 1139-1158	5.7	16
120	Tau R3-R4 Domain Dimer of the Wild Type and Phosphorylated Ser356 Sequences. I. In Solution by Atomistic Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 2975-2983	3.4	21
119	Efficacy assessment of ticagrelor versus clopidogrel in Chinese patients with acute coronary syndrome undergoing percutaneous coronary intervention by data mining and machine-learning decision tree approaches. *Journal of Clinical Pharmacy and Therapeutics*, **2020**, 45, 1076-1086	2.2	3
118	Fast, Accurate, and Reliable Protocols for Routine Calculations of Protein-Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. *ACS Omega*, **2020**, 5, 4611-4619	3.9	31
117	Novel MscL agonists that allow multiple antibiotics cytoplasmic access activate the channel through a common binding site. *PLoS ONE*, **2020**, 15, e0228153	3.7	2
116	Cryo-EM Structure of the Human Cannabinoid Receptor CB2-G Signaling Complex. *Cell*, **2020**, 180, 645-656.e13	36.2	81
115	Fast Identification of Possible Drug Treatment of Coronavirus Disease-19 (COVID-19) through Computational Drug Repurposing Study. *Journal of Chemical Information and Modeling*, **2020**, 60, 3277-3286	6.1	268
114	Fast Identification of Possible Drug Treatment of Coronavirus Disease -19 (COVID-19) Through Computational Drug Repurposing Study. *ChemRxiv*, **2020**,	4.4	9
113	Analysis of substance use and its outcomes by machine learning I. Childhood evaluation of liability to substance use disorder. *Drug and Alcohol Dependence*, **2020**, 206, 107605	4.9	14
112	Nanoparticle Conjugation of Ginsenoside Rg3 Inhibits Hepatocellular Carcinoma Development and Metastasis. *Small*, **2020**, 16, e1905233	11	30
111	How Well Does the Extended Linear Interaction Energy Method Perform in Accurate Binding Free Energy Calculations?. *Journal of Chemical Information and Modeling*, **2020**, 60, 6624-6633	6.1	4
110	Transmembrane Polar Relay Drives the Allosteric Regulation for ABCG5/G8 Sterol Transporter. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	5
109	Molecular mechanism of ultrasound interaction with a blood brain barrier model. *Journal of Chemical Physics*, **2020**, 153, 045104	3.9	5

108	Development of Cu-Based Distance Methods and Force Field Parameters for the Determination of PNA Conformations and Dynamics by EPR and MD Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 7544-7556	3.4	6
107	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. *Journal of Chemical Physics*, **2020**, 153, 114116	3.9	9
106	A fast and high-quality charge model for the next generation general AMBER force field. *Journal of Chemical Physics*, **2020**, 153, 114502	3.9	36
105	Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of A Oligomerization. *Journal of Chemical Theory and Computation*, **2020**, 16, 3920-3935	6.4	4
104	Prediction of Drug-Drug Interactions Between Opioids and Overdosed Benzodiazepines Using Physiologically Based Pharmacokinetic (PBPK) Modeling and Simulation. *Drugs in R and D*, **2019**, 19, 297-305	3.4	10
103	End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. *Chemical Reviews*, **2019**, 119, 9478-9508	68.1	449
102	An agonist of the MscL channel affects multiple bacterial species and increases membrane permeability and potency of common antibiotics. *Molecular Microbiology*, **2019**, 112, 896-905	4.1	5
101	Interaction mechanism between the focused ultrasound and lipid membrane at the molecular level. *Journal of Chemical Physics*, **2019**, 150, 215101	3.9	7
100	Structural Basis of TLR2/TLR1 Activation by the Synthetic Agonist Diprovocim. *Journal of Medicinal Chemistry*, **2019**, 62, 2938-2949	8.3	27
99	Significantly different effects of tetrahydroberberrubine enantiomers on dopamine D1/D2 receptors revealed by experimental study and integrated in silico simulation. *Journal of Computer-Aided Molecular Design*, **2019**, 33, 447-459	4.2	3
98	Structural snapshot of the cholesterol-transport ATP-binding cassette proteins. *Biochemistry and Cell Biology*, **2019**, 97, 224-233	3.6	10
97	Functional divergence caused by mutations in an energetic hotspot in ERK2. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 15514-15523	11.5	11
96	Nonequilibrium atomistic molecular dynamics simulation of tubular nanomotor propelled by bubble propulsion. *Journal of Chemical Physics*, **2019**, 151, 024103	3.9	2
95	Molecular Mechanism and Kinetics of Amyloid- Aggregate Formation: A Simulation Study. *ACS Chemical Neuroscience*, **2019**, 10, 4643-4658	5.7	5
94	Insight of Captagon Abuse by Chemogenomics Knowledgebase-guided Systems Pharmacology Target Mapping Analyses. *Scientific Reports*, **2019**, 9, 2268	4.9	7
93	New application of in silico methods in identifying mechanisms of action and key components of anti-cancer herbal formulation YIV-906 (PHY906). *Physical Chemistry Chemical Physics*, **2019**, 21, 23501-23513	3.6	5
92	Calculate protein-ligand binding affinities with the extended linear interaction energy method: application on the Cathepsin S set in the D3R Grand Challenge 3. *Journal of Computer-Aided Molecular Design*, **2019**, 33, 105-117	4.2	15
91	Development and Testing of Druglike Screening Libraries. *Journal of Chemical Information and Modeling*, **2019**, 59, 53-65	6.1	13

90	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of Aβ Dimer. *Journal of Chemical Theory and Computation*, **2019**, 15, 1440-1452	6.4	55
89	Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce ab Initio Anisotropy. *Journal of Chemical Theory and Computation*, **2019**, 15, 1146-1158	6.4	15
88	Novel compounds that specifically bind and modulate MscL: insights into channel gating mechanisms. *FASEB Journal*, **2019**, 33, 3180-3189	0.9	7
87	Molecular Mechanism of the Cell Membrane Pore Formation Induced by Bubble Stable Cavitation. *Journal of Physical Chemistry B*, **2019**, 123, 71-78	3.4	17
86	Assessing the performance of MM/PBSA and MM/GBSA methods. 8. Predicting binding free energies and poses of protein-RNA complexes. *Rna*, **2018**, 24, 1183-1194	5.8	51
85	Molecular Dynamics Simulations Revealed the Regulation of Ligands to the Interactions between Androgen Receptor and Its Coactivator. *Journal of Chemical Information and Modeling*, **2018**, 58, 1652-1661	6.1	25
84	An insight into paracetamol and its metabolites using molecular docking and molecular dynamics simulation. *Journal of Molecular Modeling*, **2018**, 24, 243	2	11
83	Breaking down cellulose fibrils with a mid-infrared laser. *Cellulose*, **2018**, 25, 5553-5568	5.5	5
82	Crystal Structures of Human Orexin 2 Receptor Bound to the Subtype-Selective Antagonist EMPA. *Structure*, **2018**, 26, 7-19.e5	5.2	41
81	Crystal structure of the human NK tachykinin receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 13264-13269	11.5	21
80	Cheminformatic Insight into the Differences between Terrestrial and Marine Originated Natural Products. *Journal of Chemical Information and Modeling*, **2018**, 58, 1182-1193	6.1	32
79	A Continuum Poisson-Boltzmann Model for Membrane Channel Proteins. *Journal of Chemical Theory and Computation*, **2017**, 13, 3398-3412	6.4	15
78	High-resolution crystal structure of the human CB1 cannabinoid receptor. *Nature*, **2016**, 540, 602-606	50.4	250
77	In Silico Chemogenomics Knowledgebase and Computational System Neuropharmacology Approach for Cannabinoid Drug Research **2016**, 183-195		2
76	Dihydrostreptomycin Directly Binds to, Modulates, and Passes through the MscL Channel Pore. *PLoS Biology*, **2016**, 14, e1002473	9.7	21
75	Crystal structure of the human sterol transporter ABCG5/ABCG8. *Nature*, **2016**, 533, 561-4	50.4	185
74	The application of in silico drug-likeness predictions in pharmaceutical research. *Advanced Drug Delivery Reviews*, **2015**, 86, 2-10	18.5	190
73	Advances in computationally modeling human oral bioavailability. *Advanced Drug Delivery Reviews*, **2015**, 86, 11-6	18.5	27

72	Molecular Dynamics Simulations of a Protein Crystal. *Bioenergetics: Open Access*, **2014**, 02,		1
71	P-loop conformation governed crizotinib resistance in G2032R-mutated ROS1 tyrosine kinase: clues from free energy landscape. *PLoS Computational Biology*, **2014**, 10, e1003729	5	77
70	MORT: a powerful foundational library for computational biology and CADD. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
69	Drug-likeness analysis of traditional Chinese medicines: 2. Characterization of scaffold architectures for drug-like compounds, non-drug-like compounds, and natural compounds from traditional Chinese medicines. *Journal of Cheminformatics*, **2013**, 5, 5	8.6	23
68	Assessing the performance of MM/PBSA and MM/GBSA methods. 3. The impact of force fields and ligand charge models. *Journal of Physical Chemistry B*, **2013**, 117, 8408-21	3.4	334
67	Accelerated conformational entropy calculations using graphic processing units. *Journal of Chemical Information and Modeling*, **2013**, 53, 2057-64	6.1	5
66	Modeling compound-target interaction network of traditional Chinese medicines for type II diabetes mellitus: insight for polypharmacology and drug design. *Journal of Chemical Information and Modeling*, **2013**, 53, 1787-803	6.1	34
65	Develop and test a solvent accessible surface area-based model in conformational entropy calculations. *Journal of Chemical Information and Modeling*, **2012**, 52, 1199-212	6.1	70
64	Development of polarizable models for molecular mechanical calculations. 3. Polarizable water models conforming to Thole polarization screening schemes. *Journal of Physical Chemistry B*, **2012**, 116, 7999-8008	3.4	42
63	Development of polarizable models for molecular mechanical calculations. 4. van der Waals parametrization. *Journal of Physical Chemistry B*, **2012**, 116, 7088-101	3.4	44
62	Drug-likeness analysis of traditional Chinese medicines: prediction of drug-likeness using machine learning approaches. *Molecular Pharmaceutics*, **2012**, 9, 2875-86	5.6	88
61	A rule-based algorithm for automatic bond type perception. *Journal of Cheminformatics*, **2012**, 4, 26	8.6	11
60	Drug-likeness analysis of traditional Chinese medicines: 1. property distributions of drug-like compounds, non-drug-like compounds and natural compounds from traditional Chinese medicines. *Journal of Cheminformatics*, **2012**, 4, 31	8.6	49
59	Challenges in Binding Free Energy Calculation using MM-PB/GBSA. *Bioenergetics: Open Access*, **2012** , 01,		2
58	ADMET evaluation in drug discovery. 11. PharmacoKinetics Knowledge Base (PKKB): a comprehensive database of pharmacokinetic and toxic properties for drugs. *Journal of Chemical Information and Modeling*, **2012**, 52, 1132-7	6.1	51
57	ADMET evaluation in drug discovery. 12. Development of binary classification models for prediction of hERG potassium channel blockage. *Molecular Pharmaceutics*, **2012**, 9, 996-1010	5.6	111
56	Assessing the performance of the MM/PBSA and MM/GBSA methods. 1. The accuracy of binding free energy calculations based on molecular dynamics simulations. *Journal of Chemical Information and Modeling*, **2011**, 51, 69-82	6.1	1511
55	Development of polarizable models for molecular mechanical calculations I: parameterization of atomic polarizability. *Journal of Physical Chemistry B*, **2011**, 115, 3091-9	3.4	114

54	ADME evaluation in drug discovery. 9. Prediction of oral bioavailability in humans based on molecular properties and structural fingerprints. *Molecular Pharmaceutics*, **2011**, 8, 841-51	5.6	83
53	Application of molecular dynamics simulations in molecular property prediction II: diffusion coefficient. *Journal of Computational Chemistry*, **2011**, 32, 3505-19	3.5	91
52	Application of Molecular Dynamics Simulations in Molecular Property Prediction I: Density and Heat of Vaporization. *Journal of Chemical Theory and Computation*, **2011**, 7, 2151-2165	6.4	85
51	Recent advances on aqueous solubility prediction. *Combinatorial Chemistry and High Throughput Screening*, **2011**, 14, 328-38	1.3	83
50	Recent developments of in silico predictions of oral bioavailability. *Combinatorial Chemistry and High Throughput Screening*, **2011**, 14, 362-74	1.3	34
49	Assessing the performance of the molecular mechanics/Poisson Boltzmann surface area and molecular mechanics/generalized Born surface area methods. II. The accuracy of ranking poses generated from docking. *Journal of Computational Chemistry*, **2011**, 32, 866-77	3.5	484
48	Correction to Application of Molecular Dynamics Simulations in Molecular Property Prediction. 1. Density and Heat of Vaporization. *Journal of Chemical Theory and Computation*, **2011**, 7, 2333	6.4	
47	Development of polarizable models for molecular mechanical calculations II: induced dipole models significantly improve accuracy of intermolecular interaction energies. *Journal of Physical Chemistry B*, **2011**, 115, 3100-11	3.4	101
46	Drug and drug candidate building block analysis. *Journal of Chemical Information and Modeling*, **2010**, 50, 55-67	6.1	83
45	Recent developments of in silico predictions of intestinal absorption and oral bioavailability. *Combinatorial Chemistry and High Throughput Screening*, **2009**, 12, 497-506	1.3	64
44	Examination of the effect of the annealing cation on higher order structures containing guanine or isoguanine repeats. *Chemistry - A European Journal*, **2009**, 15, 11244-55	4.8	22
43	Predicting drug resistance of the HIV-1 protease using molecular interaction energy components. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 837-46	4.2	72
42	Polarization effects in molecular mechanical force fields. *Journal of Physics Condensed Matter*, **2009**, 21, 333102	1.8	192
41	Aqueous solubility prediction based on weighted atom type counts and solvent accessible surface areas. *Journal of Chemical Information and Modeling*, **2009**, 49, 571-81	6.1	48
40	Chapter 5 Recent Advances on in silico ADME Modeling. *Annual Reports in Computational Chemistry*, **2009**, 101-127	1.8	18
39	Structure-ADME relationship: still a long way to go?. *Expert Opinion on Drug Metabolism and Toxicology*, **2008**, 4, 759-70	5.5	92
38	Continuum polarizable force field within the Poisson-Boltzmann framework. *Journal of Physical Chemistry B*, **2008**, 112, 7675-88	3.4	20
37	Fast approaches for molecular polarizability calculations. *Journal of Physical Chemistry A*, **2007**, 111, 4443-8	2.8	56

36	ADME evaluation in drug discovery. 7. Prediction of oral absorption by correlation and classification. *Journal of Chemical Information and Modeling*, **2007**, 47, 208-18	6.1	141
35	ADME evaluation in drug discovery. 8. The prediction of human intestinal absorption by a support vector machine. *Journal of Chemical Information and Modeling*, **2007**, 47, 2408-15	6.1	93
34	GPCR structure-based virtual screening approach for CB2 antagonist search. *Journal of Chemical Information and Modeling*, **2007**, 47, 1626-37	6.1	94
33	Gas-phase stability of G-quadruplex DNA determined by electrospray ionization tandem mass spectrometry and molecular dynamics simulations. *Journal of the American Society for Mass Spectrometry*, **2007**, 18, 1760-73	3.5	30
32	ADME evaluation in drug discovery. 6. Can oral bioavailability in humans be effectively predicted by simple molecular property-based rules?. *Journal of Chemical Information and Modeling*, **2007**, 47, 460-3	6.1	138
31	Development of reliable aqueous solubility models and their application in druglike analysis. *Journal of Chemical Information and Modeling*, **2007**, 47, 1395-404	6.1	79
30	Automatic atom type and bond type perception in molecular mechanical calculations. *Journal of Molecular Graphics and Modelling*, **2006**, 25, 247-60	2.8	3191
29	Recent Advances in Free Energy Calculations with a Combination of Molecular Mechanics and Continuum Models. *Current Computer-Aided Drug Design*, **2006**, 2, 287-306	1.4	230
28	Recent advances in computational prediction of drug absorption and permeability in drug discovery. *Current Medicinal Chemistry*, **2006**, 13, 2653-67	4.3	147
27	New-generation amber united-atom force field. *Journal of Physical Chemistry B*, **2006**, 110, 13166-76	3.4	157
26	Genetic algorithm-optimized QSPR models for bioavailability, protein binding, and urinary excretion. *Journal of Chemical Information and Modeling*, **2006**, 46, 2674-83	6.1	54
25	3D-QSAR studies of arylpyrazole antagonists of cannabinoid receptor subtypes CB1 and CB2. A combined NMR and CoMFA approach. *Journal of Medicinal Chemistry*, **2006**, 49, 625-36	8.3	55
24	Hierarchical database screenings for HIV-1 reverse transcriptase using a pharmacophore model, rigid docking, solvation docking, and MM-PB/SA. *Journal of Medicinal Chemistry*, **2005**, 48, 2432-44	8.3	64
23	Threshold dissociation and molecular modeling of transition metal complexes of flavonoids. *Journal of the American Society for Mass Spectrometry*, **2005**, 16, 139-51	3.5	45
22	Characterization of flavonoids by aluminum complexation and collisionally activated dissociation. *Journal of Mass Spectrometry*, **2005**, 40, 350-63	2.2	40
21	Identification of a specific inhibitor of the dishevelled PDZ domain. *Biochemistry*, **2005**, 44, 15495-503	3.2	172
20	Development and testing of a general amber force field. *Journal of Computational Chemistry*, **2004**, 25, 1157-74	3.5	10682
19	Discovery, modeling, and human pharmacokinetics of N-(2-acetyl-4,6-dimethylphenyl)-3-(3,4-dimethylisoxazol-5-ylsulfamoyl)thiophene-2-carboxamide (TBC3711), a second generation, ETA selective, and orally bioavailable endothelin antagonist. *Journal of Medicinal Chemistry*, **2004**, 47, 1969-86	8.3	90

18	A point-charge force field for molecular mechanics simulations of proteins based on condensed-phase quantum mechanical calculations. *Journal of Computational Chemistry*, **2003**, 24, 1999-2012	3.5	3573
17	Molecular dynamics and free energy analyses of cathepsin D-inhibitor interactions: insight into structure-based ligand design. *Journal of Medicinal Chemistry*, **2002**, 45, 1412-9	8.3	155
16	Automatic parameterization of force field by systematic search and genetic algorithms. *Journal of Computational Chemistry*, **2001**, 22, 1219-1228	3.5	112
15	Use of MM-PBSA in reproducing the binding free energies to HIV-1 RT of TIBO derivatives and predicting the binding mode to HIV-1 RT of efavirenz by docking and MM-PBSA. *Journal of the American Chemical Society*, **2001**, 123, 5221-30	16.4	616
14	Solvation Model Based on Weighted Solvent Accessible Surface Area. *Journal of Physical Chemistry B*, **2001**, 105, 5055-5067	3.4	100
13	An analysis of the interactions between the Sem-5 SH3 domain and its ligands using molecular dynamics, free energy calculations, and sequence analysis. *Journal of the American Chemical Society*, **2001**, 123, 3986-94	16.4	121
12	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. *Journal of Computational Chemistry*, **2000**, 21, 1049-1074	3.5	3321
11	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules? **2000**, 21, 1049		2
10	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules? **2000**, 21, 1049		30
9	Automated docking of peptides and proteins by using a genetic algorithm combined with a tabu search. *Protein Engineering, Design and Selection*, **1999**, 12, 639-48	1.9	40
8	Automated docking of peptides and proteins by genetic algorithm. *Chemometrics and Intelligent Laboratory Systems*, **1999**, 45, 281-286	3.8	6
7	Applications of genetic algorithms on the structure□ctivity correlation study of a group of non-nucleoside HIV-1 inhibitors. *Chemometrics and Intelligent Laboratory Systems*, **1999**, 45, 303-310	3.8	17
6	Conformational analysis of peptides using Monte Carlo simulations combined with the genetic algorithm. *Chemometrics and Intelligent Laboratory Systems*, **1999**, 45, 347-351	3.8	13
5	Applications of genetic algorithms on the structure-activity relationship analysis of some cinnamamides. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 775-81		61
4	Theoretical studies on force titration of amino-group-terminated self-assembled monolayers. *Computational and Theoretical Chemistry*, **1998**, 451, 295-303		7
3	Transmembrane polar relay drives the allosteric regulation for ABCG5/G8 sterol transporter		1
2	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?		1
1	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?		23