Junmei Wang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6992644/publications.pdf

Version: 2024-02-01

147 papers	39,265 citations	23567 58 h-index	9589 142 g-index
158 all docs	158 docs citations	158 times ranked	35401 citing authors

#	Article	IF	Citations
1	Structure and dynamics of major histocompatibility class Ib molecule H2-M3 complexed with mitochondrial-derived peptides. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10300-10312.	3.5	1
2	Recent progress in general force fields of small molecules. Current Opinion in Structural Biology, 2022, 72, 187-193.	5.7	15
3	Development and Evaluation of Geometry Optimization Algorithms in Conjunction with ANI Potentials. Journal of Chemical Theory and Computation, 2022, 18, 978-991.	5.3	2
4	In Silico Prediction and Validation of CB2 Allosteric Binding Sites to Aid the Design of Allosteric Modulators. Molecules, 2022, 27, 453.	3.8	14
5	A multiple-step in silico screening protocol to identify allosteric inhibitors of Spikeâ€“hACE2 binding. Physical Chemistry Chemical Physics, 2022, 24, 4305-4316.	2.8	6
6	Elastic moduli of normal and cancer cell membranes revealed by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2022, 24, 6225-6237.	2.8	10
7	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.	1.6	1
8	In Silico Screen Identifies a New Family of Agonists for the Bacterial Mechanosensitive Channel MscL. Antibiotics, 2022, 11, 433.	3.7	4
9	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.	7.1	4
10	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.	2.5	1
11	Joint Computational/Cell-Based Approach for Screening Inhibitors of Tau Oligomerization: A Proof-of-Concept Study. Journal of Alzheimer's Disease, 2022, 89, 107-119.	2.6	2
12	Landscape of drug-resistance mutations in kinase regulatory hotspots. Briefings in Bioinformatics, 2021, 22, .	6.5	15
13	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.	5.3	16
14	Nonequilibrium molecular dynamics simulations of infrared laser-induced dissociation of a tetrameric AÎ²42 Î²-barrel in a neuronal membrane model. Chemistry and Physics of Lipids, 2021, 234, 105030.	3.2	2
15	Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. Journal of Cheminformatics, 2021, 13, 11.	6.1	1
16	Machine learning on ligand-residue interaction profiles to significantly improve binding affinity prediction. Briefings in Bioinformatics, 2021, 22, .	6.5	17
17	VAD-MM/GBSA: A Variable Atomic Dielectric MM/GBSA Model for Improved Accuracy in Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2844-2856.	5.4	29
18	In silico binding profile characterization of SARS-CoV-2 spike protein and its mutants bound to human ACE2 receptor. Briefings in Bioinformatics, 2021, 22, .	6.5	22

#	Article	IF	Citations
19	Drugâ€“Drug Interaction Between Oxycodone and Diazepam by a Combined in Silico Pharmacokinetic and Pharmacodynamic Modeling Approach. ACS Chemical Neuroscience, 2021, 12, 1777-1790.	3.5	5
20	Molecular Mechanism of Ultrasound-Induced Structural Defects in Liposomes: A Nonequilibrium Molecular Dynamics Simulation Study. Langmuir, 2021, 37, 7945-7954.	3.5	5
21	Sulfatides are endogenous ligands for the TLR4â€“MD-2 complex. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	24
22	Aicardi-GoutiÃ¨res syndrome-associated mutation at ADAR1 gene locus activates innate immune response in mouse brain. Journal of Neuroinflammation, 2021, 18, 169.	7.2	25
23	TMEM120A is a coenzyme A-binding membrane protein with structural similarities to ELOVL fatty acid elongase. ELife, 2021, 10, .	6.0	20
24	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.	5.3	23
25	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.	3.2	26
26	Nanoparticle Conjugation of Ginsenoside Rg3 Inhibits Hepatocellular Carcinoma Development and Metastasis. Small, 2020, 16, e1905233.	10.0	72
27	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.	5.4	9
28	Transmembrane Polar Relay Drives the Allosteric Regulation for ABCG5/G8 Sterol Transporter. International Journal of Molecular Sciences, 2020, 21, 8747.	4.1	8
29	Molecular mechanism of ultrasound interaction with a blood brain barrier model. Journal of Chemical Physics, 2020, 153, 045104.	3.0	15
30	Development of Cu²⁺-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.	2.6	12
31	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. Journal of Chemical Physics, 2020, 153, 114116.	3.0	19
32	A fast and high-quality charge model for the next generation general AMBER force field. Journal of Chemical Physics, 2020, 153, 114502.	3.0	195
33	Orientation and dynamics of Cu²⁺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.	2.8	10
34	Infrared Laser-Induced Amyloid Fibril Dissociation: A Joint Experimental/Theoretical Study on the GNNQQNY Peptide. Journal of Physical Chemistry B, 2020, 124, 6266-6277.	2.6	16
35	Development and Evaluation of MM/GBSA Based on a Variable Dielectric GB Model for Predicting Proteinâ€“Ligand Binding Affinities. Journal of Chemical Information and Modeling, 2020, 60, 5353-5365.	5.4	25
36	Molecular Dynamics Simulations Based on Newly Developed Force Field Parameters for Cu²⁺ Spin Labels Provide Insights into Double-Histidine-Based Double Electronâ€“Electron Resonance. Journal of Physical Chemistry B, 2020, 124, 2788-2797.	2.6	32

#	Article	IF	Citations
37	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.	3.5	38
38	Tau R3â€“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.	2.6	30
39	Efficacy assessment of ticagrelor versus clopidogrel in Chinese patients with acute coronary syndrome undergoing percutaneous coronary intervention by data mining and machineâ€learning decision tree approaches. Journal of Clinical Pharmacy and Therapeutics, 2020, 45, 1076-1086.	1.5	9
40	Fast, Accurate, and Reliable Protocols for Routine Calculations of Proteinâ€“Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. ACS Omega, 2020, 5, 4611-4619.	3.5	74
41	Novel MscL agonists that allow multiple antibiotics cytoplasmic access activate the channel through a common binding site. PLoS ONE, 2020, 15, e0228153.	2.5	14
42	Cryo-EM Structure of the Human Cannabinoid Receptor CB2-Gi Signaling Complex. Cell, 2020, 180, 645-654.e13.	28.9	167
43	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.	5.4	373
44	Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of AÎ² Oligomerization. Journal of Chemical Theory and Computation, 2020, 16, 3920-3935.	5.3	7
45	Structural snapshot of the cholesterol-transport ATP-binding cassette proteins. Biochemistry and Cell Biology, 2019, 97, 224-233.	2.0	14
46	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.	7.1	23
47	Nonequilibrium atomistic molecular dynamics simulation of tubular nanomotor propelled by bubble propulsion. Journal of Chemical Physics, 2019, 151, 024103.	3.0	4
48	Molecular Mechanism and Kinetics of Amyloid-Î²₄₂ Aggregate Formation: A Simulation Study. ACS Chemical Neuroscience, 2019, 10, 4643-4658.	3.5	13
49	Prediction of Drugâ€“Drug Interactions Between Opioids and Overdosed Benzodiazepines Using Physiologically Based Pharmacokinetic (PBPK) Modeling and Simulation. Drugs in R and D, 2019, 19, 297-305.	2.2	17
50	End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. Chemical Reviews, 2019, 119, 9478-9508.	47.7	1,064
51	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.	2.5	16
52	Interaction mechanism between the focused ultrasound and lipid membrane at the molecular level. Journal of Chemical Physics, 2019, 150, 215101.	3.0	11
53	Structural Basis of TLR2/TLR1 Activation by the Synthetic Agonist Diprovocim. Journal of Medicinal Chemistry, 2019, 62, 2938-2949.	6.4	53
54	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.	2.9	6

#	Article	IF	Citations
55	Insight of Captagon Abuse by Chemogenomics Knowledgebase-guided Systems Pharmacology Target Mapping Analyses. Scientific Reports, 2019, 9, 2268.	3.3	10
56	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.	2.8	9
57	Calculate proteinâ€“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.	2.9	27
58	Development and Testing of Druglike Screening Libraries. Journal of Chemical Information and Modeling, 2019, 59, 53-65.	5.4	22
59	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of Aî²_{16â€“22} Dimer. Journal of Chemical Theory and Computation, 2019, 15, 1440-1452.	5.3	102
60	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.	5.3	26
61	Novel compounds that specifically bind and modulate MscL: insights into channel gating mechanisms. FASEB Journal, 2019, 33, 3180-3189.	0.5	17
62	Molecular Mechanism of the Cell Membrane Pore Formation Induced by Bubble Stable Cavitation. Journal of Physical Chemistry B, 2019, 123, 71-78.	2.6	25
63	Crystal Structures of Human Orexin 2 Receptor Bound to the Subtype-Selective Antagonist EMPA. Structure, 2018, 26, 7-19.e5.	3.3	55
64	Crystal structure of the human NK ₁ tachykinin receptor. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 13264-13269.	7.1	30
65	Cheminformatic Insight into the Differences between Terrestrial and Marine Originated Natural Products. Journal of Chemical Information and Modeling, 2018, 58, 1182-1193.	5.4	45
66	Assessing the performance of MM/PBSA and MM/GBSA methods. 8. Predicting binding free energies and poses of proteinâ€“RNA complexes. Rna, 2018, 24, 1183-1194.	3.5	84
67	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.	5.4	37
68	An insight into paracetamol and its metabolites using molecular docking and molecular dynamics simulation. Journal of Molecular Modeling, 2018, 24, 243.	1.8	14
69	Breaking down cellulose fibrils with a mid-infrared laser. Cellulose, 2018, 25, 5553-5568.	4.9	8
70	A Continuum Poissonâ€“Boltzmann Model for Membrane Channel Proteins. Journal of Chemical Theory and Computation, 2017, 13, 3398-3412.	5.3	19
71	Dihydrostreptomycin Directly Binds to, Modulates, and Passes through the MscL Channel Pore. PLoS Biology, 2016, 14, e1002473.	5.6	35
72	Crystal structure of the human sterol transporter ABCG5/ABCG8. Nature, 2016, 533, 561-564.	27.8	233

#	Article	IF	Citations
73	High-resolution crystal structure of the human CB1 cannabinoid receptor. Nature, 2016, 540, 602-606.	27.8	345
74	In Silico Chemogenomics Knowledgebase and Computational System Neuropharmacology Approach for Cannabinoid Drug Research. , 2016, , 183-195.		8
75	The application of in silico drug-likeness predictions in pharmaceutical research. Advanced Drug Delivery Reviews, 2015, 86, 2-10.	13.7	306
76	Advances in computationally modeling human oral bioavailability. Advanced Drug Delivery Reviews, 2015, 86, 11-16.	13.7	36
77	Molecular Dynamics Simulations of a Protein Crystal. Bioenergetics: Open Access, 2014, 02, .	0.1	1
78	P-loop Conformation Governed Crizotinib Resistance in G2032R-Mutated ROS1 Tyrosine Kinase: Clues from Free Energy Landscape. PLoS Computational Biology, 2014, 10, e1003729.	3.2	86
79	MORT: a powerful foundational library for computational biology and CADD. Journal of Cheminformatics, 2014, 6, .	6.1	0
80	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.	6.1	25
81	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, 8408-8421.	2.6	419
82	Accelerated Conformational Entropy Calculations Using Graphic Processing Units. Journal of Chemical Information and Modeling, 2013, 53, 2057-2064.	5.4	6
83	Modeling Compoundâ€“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, 1787-1803.	5.4	39
84	Develop and Test a Solvent Accessible Surface Area-Based Model in Conformational Entropy Calculations. Journal of Chemical Information and Modeling, 2012, 52, 1199-1212.	5.4	99
85	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.	2.6	49
86	Development of Polarizable Models for Molecular Mechanical Calculations. 4. van der Waals Parametrization. Journal of Physical Chemistry B, 2012, 116, 7088-7101.	2.6	60
87	Drug-likeness Analysis of Traditional Chinese Medicines: Prediction of Drug-likeness Using Machine Learning Approaches. Molecular Pharmaceutics, 2012, 9, 2875-2886.	4.6	96
88	A rule-based algorithm for automatic bond type perception. Journal of Cheminformatics, 2012, 4, 26.	6.1	15
89	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.	6.1	63
90	Challenges in Binding Free Energy Calculation using MM-PB/GBSA. Bioenergetics: Open Access, 2012, 01, .	0.1	3

#	Article	IF	Citations
91	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, 1132-1137.	5.4	62
92	ADMET Evaluation in Drug Discovery. 12. Development of Binary Classification Models for Prediction of hERG Potassium Channel Blockage. Molecular Pharmaceutics, 2012, 9, 996-1010.	4.6	137
93	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, 2333-2333.	5.3	0
94	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, 3100-3111.	2.6	116
95	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.	5.4	2,005
96	Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability. Journal of Physical Chemistry B, 2011, 115, 3091-3099.	2.6	137
97	ADME Evaluation in Drug Discovery. 9. Prediction of Oral Bioavailability in Humans Based on Molecular Properties and Structural Fingerprints. Molecular Pharmaceutics, 2011, 8, 841-851.	4.6	114
98	Application of molecular dynamics simulations in molecular property prediction II: Diffusion coefficient. Journal of Computational Chemistry, 2011, 32, 3505-3519.	3.3	135
99	Application of Molecular Dynamics Simulations in Molecular Property Prediction. 1. Density and Heat of Vaporization. Journal of Chemical Theory and Computation, 2011, 7, 2151-2165.	5.3	114
100	Recent Advances on Aqueous Solubility Prediction. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 328-338.	1.1	102
101	Recent Developments of In Silico Predictions of Oral Bioavailability. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 362-374.	1.1	38
102	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, 866-877.	3.3	615
103	Drug and Drug Candidate Building Block Analysis. Journal of Chemical Information and Modeling, 2010, 50, 55-67.	5.4	96
104	Recent Developments of In Silico Predictions of Intestinal Absorption and Oral Bioavailability. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 497-506.	1.1	74
105	Examination of the Effect of the Annealing Cation on Higher Order Structures Containing Guanine or Isoguanine Repeats. Chemistry - A European Journal, 2009, 15, 11244-11255.	3.3	23
106	Predicting drug resistance of the HIVâ€1 protease using molecular interaction energy components. Proteins: Structure, Function and Bioinformatics, 2009, 74, 837-846.	2.6	78
107	Polarization effects in molecular mechanical force fields. Journal of Physics Condensed Matter, 2009, 21, 333102.	1.8	236
108	Aqueous Solubility Prediction Based on Weighted Atom Type Counts and Solvent Accessible Surface Areas. Journal of Chemical Information and Modeling, 2009, 49, 571-581.	5.4	61

#	Article	IF	Citations
109	Chapter 5 Recent Advances on in silico ADME Modeling. Annual Reports in Computational Chemistry, 2009, , 101-127.	1.7	21
110	Structure â€“ ADME relationship: still a long way to go?. Expert Opinion on Drug Metabolism and Toxicology, 2008, 4, 759-770.	3.3	120
111	Continuum Polarizable Force Field within the Poissonâ^'Boltzmann Framework. Journal of Physical Chemistry B, 2008, 112, 7675-7688.	2.6	26
112	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, 460-463.	5.4	155
113	Development of Reliable Aqueous Solubility Models and Their Application in Druglike Analysis. Journal of Chemical Information and Modeling, 2007, 47, 1395-1404.	5.4	103
114	Fast Approaches for Molecular Polarizability Calculations. Journal of Physical Chemistry A, 2007, 111, 4443-4448.	2.5	65
115	ADME Evaluation in Drug Discovery. 7. Prediction of Oral Absorption by Correlation and Classification. Journal of Chemical Information and Modeling, 2007, 47, 208-218.	5.4	171
116	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, 2408-2415.	5.4	114
117	GPCR Structure-Based Virtual Screening Approach for CB2 Antagonist Search. Journal of Chemical Information and Modeling, 2007, 47, 1626-1637.	5.4	103
118	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, 1760-1773.	2.8	33
119	New-Generation Amber United-Atom Force Field. Journal of Physical Chemistry B, 2006, 110, 13166-13176.	2.6	176
120	Genetic Algorithm-Optimized QSPR Models for Bioavailability, Protein Binding, and Urinary Excretion. Journal of Chemical Information and Modeling, 2006, 46, 2674-2683.	5.4	60
121	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, 625-636.	6.4	59
122	Automatic atom type and bond type perception in molecular mechanical calculations. Journal of Molecular Graphics and Modelling, 2006, 25, 247-260.	2.4	4,173
123	Recent Advances in Free Energy Calculations with a Combination of Molecular Mechanics and Continuum Models. Current Computer-Aided Drug Design, 2006, 2, 287-306.	1.2	300
124	Recent Advances in Computational Prediction of Drug Absorption and Permeability in Drug Discovery. Current Medicinal Chemistry, 2006, 13, 2653-2667.	2.4	167
125	Threshold dissociation and molecular modeling of transition metal complexes of flavonoids. Journal of the American Society for Mass Spectrometry, 2005, 16, 139-151.	2.8	48
126	Characterization of flavonoids by aluminum complexation and collisionally activated dissociation. Journal of Mass Spectrometry, 2005, 40, 350-363.	1.6	48

#	Article	IF	Citations
127	Identification of a Specific Inhibitor of the Dishevelled PDZ Domainâ€. Biochemistry, 2005, 44, 15495-15503.	2.5	193
128	Hierarchical Database Screenings for HIV-1 Reverse Transcriptase Using a Pharmacophore Model, Rigid Docking, Solvation Docking, and MMâ^'PB/SA. Journal of Medicinal Chemistry, 2005, 48, 2432-2444.	6.4	67
129	Development and testing of a general amber force field. Journal of Computational Chemistry, 2004, 25, 1157-1174.	3.3	14,342
130	Discovery, Modeling, and Human Pharmacokinetics ofN-(2-Acetyl-4,6-dimethylphenyl)-3-(3,4-dimethylisoxazol-5-ylsulfamoyl)thiophene-2-carboxamide (TBC3711), a Second Generation, ETASelective, and Orally Bioavailable Endothelin Antagonist1. Journal of Medicinal Chemistry, 2004, 47, 1969-1986.	6.4	102
131	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.	3.3	4,028
132	Molecular Dynamics and Free Energy Analyses of Cathepsin Dâ^'Inhibitor Interactions:â€‰ Insight into Structure-Based Ligand Design. Journal of Medicinal Chemistry, 2002, 45, 1412-1419.	6.4	168
133	Solvation Model Based on Weighted Solvent Accessible Surface Area. Journal of Physical Chemistry B, 2001, 105, 5055-5067.	2.6	107
134	An Analysis of the Interactions between the Semâ^'5 SH3 Domain and Its Ligands Using Molecular Dynamics, Free Energy Calculations, and Sequence Analysis. Journal of the American Chemical Society, 2001, 123, 3986-3994.	13.7	130
135	Automatic parameterization of force field by systematic search and genetic algorithms. Journal of Computational Chemistry, 2001, 22, 1219-1228.	3.3	122
136	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, 5221-5230.	13.7	676
137	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.	3.3	3,725
138	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. , 2000, 21, 1049.		2
139	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.	3.3	32
140	Automated docking of peptides and proteins by using a genetic algorithm combined with a tabu search. Protein Engineering, Design and Selection, 1999, 12, 639-648.	2.1	48
141	Automated docking of peptides and proteins by genetic algorithm. Chemometrics and Intelligent Laboratory Systems, 1999, 45, 281-286.	3.5	7
142	Applications of genetic algorithms on the structureâ€“activity correlation study of a group of non-nucleoside HIV-1 inhibitors. Chemometrics and Intelligent Laboratory Systems, 1999, 45, 303-310.	3.5	21
143	Conformational analysis of peptides using Monte Carlo simulations combined with the genetic algorithm. Chemometrics and Intelligent Laboratory Systems, 1999, 45, 347-351.	3.5	13
144	Applications of Genetic Algorithms on the Structureâ^'Activity Relationship Analysis of Some Cinnamamides. Journal of Chemical Information and Computer Sciences, 1999, 39, 775-781.	2.8	63

#	Article	IF	Citations
145	Theoretical studies on force titration of amino-group-terminated self-assembled monolayers. Computational and Theoretical Chemistry, 1998, 451, 295-303.	1.5	9
146	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. , 0, .		1
147	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. , 0, .		25