

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	Development and testing of a general amber force field. <i>Journal of Computational Chemistry</i> , 2004, 25, 1157-1174.	3.3	14,342
2	Automatic atom type and bond type perception in molecular mechanical calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2006, 25, 247-260.	2.4	4,173
3	A point-charge force field for molecular mechanics simulations of proteins based on condensed-phase quantum mechanical calculations. <i>Journal of Computational Chemistry</i> , 2003, 24, 1999-2012.	3.3	4,028
4	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. <i>Journal of Computational Chemistry</i> , 2000, 21, 1049-1074.	3.3	3,725
5	Assessing the Performance of the MM/PBSA and MM/GBSA Methods. 1. The Accuracy of Binding Free Energy Calculations Based on Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 69-82.	5.4	2,005
6	End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. <i>Chemical Reviews</i> , 2019, 119, 9478-9508.	47.7	1,064
7	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. <i>Journal of the American Chemical Society</i> , 2001, 123, 5221-5230.	13.7	676
8	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. <i>Journal of Computational Chemistry</i> , 2011, 32, 866-877.	3.3	615
9	Assessing the Performance of MM/PBSA and MM/GBSA Methods. 3. The Impact of Force Fields and Ligand Charge Models. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8408-8421.	2.6	419
10	Fast Identification of Possible Drug Treatment of Coronavirus Disease-19 (COVID-19) through Computational Drug Repurposing Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3277-3286.	5.4	373
11	High-resolution crystal structure of the human CB1 cannabinoid receptor. <i>Nature</i> , 2016, 540, 602-606.	27.8	345
12	The application of in silico drug-likeness predictions in pharmaceutical research. <i>Advanced Drug Delivery Reviews</i> , 2015, 86, 2-10.	13.7	306
13	Recent Advances in Free Energy Calculations with a Combination of Molecular Mechanics and Continuum Models. <i>Current Computer-Aided Drug Design</i> , 2006, 2, 287-306.	1.2	300
14	Polarization effects in molecular mechanical force fields. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 333102.	1.8	236
15	Crystal structure of the human sterol transporter ABCG5/ABCG8. <i>Nature</i> , 2016, 533, 561-564.	27.8	233
16	A fast and high-quality charge model for the next generation general AMBER force field. <i>Journal of Chemical Physics</i> , 2020, 153, 114502.	3.0	195
17	Identification of a Specific Inhibitor of the Dishevelled PDZ Domain. <i>Biochemistry</i> , 2005, 44, 15495-15503.	2.5	193
18	New-Generation Amber United-Atom Force Field. <i>Journal of Physical Chemistry B</i> , 2006, 110, 13166-13176.	2.6	176

#	ARTICLE	IF	CITATIONS
19	ADME Evaluation in Drug Discovery. 7. Prediction of Oral Absorption by Correlation and Classification. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 208-218.	5.4	171
20	Molecular Dynamics and Free Energy Analyses of Cathepsin Dâ”Inhibitor Interactions:â€‰ Insight into Structure-Based Ligand Design. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 1412-1419.	6.4	168
21	Recent Advances in Computational Prediction of Drug Absorption and Permeability in Drug Discovery. <i>Current Medicinal Chemistry</i> , 2006, 13, 2653-2667.	2.4	167
22	Cryo-EM Structure of the Human Cannabinoid Receptor CB2-Gi Signaling Complex. <i>Cell</i> , 2020, 180, 645-654.e13.	28.9	167
23	ADME Evaluation in Drug Discovery. 6. Can Oral Bioavailability in Humans Be Effectively Predicted by Simple Molecular Property-Based Rules?. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 460-463.	5.4	155
24	Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3091-3099.	2.6	137
25	ADMET Evaluation in Drug Discovery. 12. Development of Binary Classification Models for Prediction of hERG Potassium Channel Blockage. <i>Molecular Pharmaceutics</i> , 2012, 9, 996-1010.	4.6	137
26	Application of molecular dynamics simulations in molecular property prediction II: Diffusion coefficient. <i>Journal of Computational Chemistry</i> , 2011, 32, 3505-3519.	3.3	135
27	An Analysis of the Interactions between the Semâ”5 SH3 Domain and Its Ligands Using Molecular Dynamics, Free Energy Calculations, and Sequence Analysis. <i>Journal of the American Chemical Society</i> , 2001, 123, 3986-3994.	13.7	130
28	Automatic parameterization of force field by systematic search and genetic algorithms. <i>Journal of Computational Chemistry</i> , 2001, 22, 1219-1228.	3.3	122
29	Structure â€” ADME relationship: still a long way to go?. <i>Expert Opinion on Drug Metabolism and Toxicology</i> , 2008, 4, 759-770.	3.3	120
30	Development of Polarizable Models for Molecular Mechanical Calculations II: Induced Dipole Models Significantly Improve Accuracy of Intermolecular Interaction Energies. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3100-3111.	2.6	116
31	ADME Evaluation in Drug Discovery. 8. The Prediction of Human Intestinal Absorption by a Support Vector Machine. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2408-2415.	5.4	114
32	ADME Evaluation in Drug Discovery. 9. Prediction of Oral Bioavailability in Humans Based on Molecular Properties and Structural Fingerprints. <i>Molecular Pharmaceutics</i> , 2011, 8, 841-851.	4.6	114
33	Application of Molecular Dynamics Simulations in Molecular Property Prediction. 1. Density and Heat of Vaporization. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2151-2165.	5.3	114
34	Solvation Model Based on Weighted Solvent Accessible Surface Area. <i>Journal of Physical Chemistry B</i> , 2001, 105, 5055-5067.	2.6	107
35	Development of Reliable Aqueous Solubility Models and Their Application in Druglike Analysis. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1395-1404.	5.4	103
36	GPCR Structure-Based Virtual Screening Approach for CB2 Antagonist Search. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1626-1637.	5.4	103

#	ARTICLE	IF	CITATIONS
37	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, ETASelective, and Orally Bioavailable Endothelin Antagonist. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 1969-1986.	6.4	102
38	Recent Advances on Aqueous Solubility Prediction. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2011, 14, 328-338.	1.1	102
39	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of A β Dimer. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1440-1452.	5.3	102
40	Develop and Test a Solvent Accessible Surface Area-Based Model in Conformational Entropy Calculations. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1199-1212.	5.4	99
41	Drug and Drug Candidate Building Block Analysis. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 55-67.	5.4	96
42	Drug-likeness Analysis of Traditional Chinese Medicines: Prediction of Drug-likeness Using Machine Learning Approaches. <i>Molecular Pharmaceutics</i> , 2012, 9, 2875-2886.	4.6	96
43	P-loop Conformation Governed Crizotinib Resistance in G2032R-Mutated ROS1 Tyrosine Kinase: Clues from Free Energy Landscape. <i>PLoS Computational Biology</i> , 2014, 10, e1003729.	3.2	86
44	Assessing the performance of MM/PBSA and MM/GBSA methods. 8. Predicting binding free energies and poses of protein-RNA complexes. <i>Rna</i> , 2018, 24, 1183-1194.	3.5	84
45	Predicting drug resistance of the HIV-1 protease using molecular interaction energy components. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 74, 837-846.	2.6	78
46	Recent Developments of In Silico Predictions of Intestinal Absorption and Oral Bioavailability. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009, 12, 497-506.	1.1	74
47	Fast, Accurate, and Reliable Protocols for Routine Calculations of Protein-Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. <i>ACS Omega</i> , 2020, 5, 4611-4619.	3.5	74
48	Nanoparticle Conjugation of Ginsenoside Rg3 Inhibits Hepatocellular Carcinoma Development and Metastasis. <i>Small</i> , 2020, 16, e1905233.	10.0	72
49	Hierarchical Database Screenings for HIV-1 Reverse Transcriptase Using a Pharmacophore Model, Rigid Docking, Solvation Docking, and MM-PB/SA. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 2432-2444.	6.4	67
50	Fast Approaches for Molecular Polarizability Calculations. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4443-4448.	2.5	65
51	Applications of Genetic Algorithms on the Structure-Activity Relationship Analysis of Some Cinnamamides. <i>Journal of Chemical Information and Computer Sciences</i> , 1999, 39, 775-781.	2.8	63
52	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. <i>Journal of Cheminformatics</i> , 2012, 4, 31.	6.1	63
53	ADMET Evaluation in Drug Discovery. 11. Pharmacokinetics Knowledge Base (PKKB): A Comprehensive Database of Pharmacokinetic and Toxic Properties for Drugs. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1132-1137.	5.4	62
54	Aqueous Solubility Prediction Based on Weighted Atom Type Counts and Solvent Accessible Surface Areas. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 571-581.	5.4	61

#	ARTICLE	IF	CITATIONS
55	Genetic Algorithm-Optimized QSPR Models for Bioavailability, Protein Binding, and Urinary Excretion. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 2674-2683.	5.4	60
56	Development of Polarizable Models for Molecular Mechanical Calculations. 4. van der Waals Parametrization. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7088-7101.	2.6	60
57	3D-QSAR Studies of Arylpyrazole Antagonists of Cannabinoid Receptor Subtypes CB1 and CB2. A Combined NMR and CoMFA Approach. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 625-636.	6.4	59
58	Crystal Structures of Human Orexin 2 Receptor Bound to the Subtype-Selective Antagonist EMPA. <i>Structure</i> , 2018, 26, 7-19.e5.	3.3	55
59	Structural Basis of TLR2/TLR1 Activation by the Synthetic Agonist Diprovocim. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 2938-2949.	6.4	53
60	Development of Polarizable Models for Molecular Mechanical Calculations. 3. Polarizable Water Models Conforming to Thole Polarization Screening Schemes. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7999-8008.	2.6	49
61	Automated docking of peptides and proteins by using a genetic algorithm combined with a tabu search. <i>Protein Engineering, Design and Selection</i> , 1999, 12, 639-648.	2.1	48
62	Threshold dissociation and molecular modeling of transition metal complexes of flavonoids. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 139-151.	2.8	48
63	Characterization of flavonoids by aluminum complexation and collisionally activated dissociation. <i>Journal of Mass Spectrometry</i> , 2005, 40, 350-363.	1.6	48
64	Cheminformatic Insight into the Differences between Terrestrial and Marine Originated Natural Products. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1182-1193.	5.4	45
65	Modeling Compound-Target Interaction Network of Traditional Chinese Medicines for Type II Diabetes Mellitus: Insight for Polypharmacology and Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1787-1803.	5.4	39
66	Recent Developments of In Silico Predictions of Oral Bioavailability. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2011, 14, 362-374.	1.1	38
67	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. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1139-1158.	3.5	38
68	Molecular Dynamics Simulations Revealed the Regulation of Ligands to the Interactions between Androgen Receptor and Its Coactivator. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1652-1661.	5.4	37
69	Advances in computationally modeling human oral bioavailability. <i>Advanced Drug Delivery Reviews</i> , 2015, 86, 11-16.	13.7	36
70	Dihydrostreptomycin Directly Binds to, Modulates, and Passes through the MscL Channel Pore. <i>PLoS Biology</i> , 2016, 14, e1002473.	5.6	35
71	Gas-phase stability of G-quadruplex DNA determined by electrospray ionization tandem mass spectrometry and molecular dynamics simulations. <i>Journal of the American Society for Mass Spectrometry</i> , 2007, 18, 1760-1773.	2.8	33
72	Molecular Dynamics Simulations Based on Newly Developed Force Field Parameters for Cu ²⁺ Spin Labels Provide Insights into Double-Histidine-Based Double Electron-Electron Resonance. <i>Journal of Physical Chemistry B</i> , 2020, 124, 2788-2797.	2.6	32

#	ARTICLE	IF	CITATIONS
73	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
74	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
75	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.	2.6	30
76	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.	5.4	29
77	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.	2.9	27
78	Continuum Polarizable Force Field within the Poisson-Boltzmann Framework. Journal of Physical Chemistry B, 2008, 112, 7675-7688.	2.6	26
79	Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce <i>ab Initio</i> Anisotropy. Journal of Chemical Theory and Computation, 2019, 15, 1146-1158.	5.3	26
80	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
81	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
82	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
83	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.	5.4	25
84	Aicardi-Goutières syndrome-associated mutation at ADAR1 gene locus activates innate immune response in mouse brain. Journal of Neuroinflammation, 2021, 18, 169.	7.2	25
85	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. , 0, .		25
86	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, .	7.1	24
87	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
88	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
89	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
90	Development and Testing of Druglike Screening Libraries. Journal of Chemical Information and Modeling, 2019, 59, 53-65.	5.4	22

#	ARTICLE	IF	CITATIONS
91	<i>In silico</i> binding profile characterization of SARS-CoV-2 spike protein and its mutants bound to human ACE2 receptor. <i>Briefings in Bioinformatics</i> , 2021, 22, .	6.5	22
92	Applications of genetic algorithms on the structure-activity correlation study of a group of non-nucleoside HIV-1 inhibitors. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1999, 45, 303-310.	3.5	21
93	Chapter 5 Recent Advances on <i>in silico</i> ADME Modeling. <i>Annual Reports in Computational Chemistry</i> , 2009, , 101-127.	1.7	21
94	TMEM120A is a coenzyme A-binding membrane protein with structural similarities to ELOVL fatty acid elongase. <i>ELife</i> , 2021, 10, .	6.0	20
95	A Continuum Poisson-Boltzmann Model for Membrane Channel Proteins. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3398-3412.	5.3	19
96	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. <i>Journal of Chemical Physics</i> , 2020, 153, 114116.	3.0	19
97	Prediction of Drug-Drug Interactions Between Opioids and Overdosed Benzodiazepines Using Physiologically Based Pharmacokinetic (PBPK) Modeling and Simulation. <i>Drugs in R and D</i> , 2019, 19, 297-305.	2.2	17
98	Novel compounds that specifically bind and modulate MscL: insights into channel gating mechanisms. <i>FASEB Journal</i> , 2019, 33, 3180-3189.	0.5	17
99	Machine learning on ligand-residue interaction profiles to significantly improve binding affinity prediction. <i>Briefings in Bioinformatics</i> , 2021, 22, .	6.5	17
100	An agonist of the MscL channel affects multiple bacterial species and increases membrane permeability and potency of common antibiotics. <i>Molecular Microbiology</i> , 2019, 112, 896-905.	2.5	16
101	Infrared Laser-Induced Amyloid Fibril Dissociation: A Joint Experimental/Theoretical Study on the GNNQQNY Peptide. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6266-6277.	2.6	16
102	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1086-1097.	5.3	16
103	A rule-based algorithm for automatic bond type perception. <i>Journal of Cheminformatics</i> , 2012, 4, 26.	6.1	15
104	Molecular mechanism of ultrasound interaction with a blood brain barrier model. <i>Journal of Chemical Physics</i> , 2020, 153, 045104.	3.0	15
105	Landscape of drug-resistance mutations in kinase regulatory hotspots. <i>Briefings in Bioinformatics</i> , 2021, 22, .	6.5	15
106	Recent progress in general force fields of small molecules. <i>Current Opinion in Structural Biology</i> , 2022, 72, 187-193.	5.7	15
107	An insight into paracetamol and its metabolites using molecular docking and molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2018, 24, 243.	1.8	14
108	Structural snapshot of the cholesterol-transport ATP-binding cassette proteins. <i>Biochemistry and Cell Biology</i> , 2019, 97, 224-233.	2.0	14

#	ARTICLE	IF	CITATIONS
109	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
110	In Silico Prediction and Validation of CB2 Allosteric Binding Sites to Aid the Design of Allosteric Modulators. Molecules, 2022, 27, 453.	3.8	14
111	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
112	Molecular Mechanism and Kinetics of Amyloid- β_{42} Aggregate Formation: A Simulation Study. ACS Chemical Neuroscience, 2019, 10, 4643-4658.	3.5	13
113	Development of Cu ²⁺ -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
114	Interaction mechanism between the focused ultrasound and lipid membrane at the molecular level. Journal of Chemical Physics, 2019, 150, 215101.	3.0	11
115	Insight of Captagon Abuse by Chemogenomics Knowledgebase-guided Systems Pharmacology Target Mapping Analyses. Scientific Reports, 2019, 9, 2268.	3.3	10
116	Orientation and dynamics of Cu ²⁺ -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
117	Elastic moduli of normal and cancer cell membranes revealed by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2022, 24, 6225-6237.	2.8	10
118	Theoretical studies on force titration of amino-group-terminated self-assembled monolayers. Computational and Theoretical Chemistry, 1998, 451, 295-303.	1.5	9
119	New application of <i>in silico</i> 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
120	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
121	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.	1.5	9
122	Breaking down cellulose fibrils with a mid-infrared laser. Cellulose, 2018, 25, 5553-5568.	4.9	8
123	Transmembrane Polar Relay Drives the Allosteric Regulation for ABCG5/G8 Sterol Transporter. International Journal of Molecular Sciences, 2020, 21, 8747.	4.1	8
124	In Silico Chemogenomics Knowledgebase and Computational System Neuropharmacology Approach for Cannabinoid Drug Research. , 2016, , 183-195.		8
125	Automated docking of peptides and proteins by genetic algorithm. Chemometrics and Intelligent Laboratory Systems, 1999, 45, 281-286.	3.5	7
126	Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of A β Oligomerization. Journal of Chemical Theory and Computation, 2020, 16, 3920-3935.	5.3	7

#	ARTICLE	IF	CITATIONS
127	Accelerated Conformational Entropy Calculations Using Graphic Processing Units. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2057-2064.	5.4	6
128	Significantly different effects of tetrahydroberberrubine enantiomers on dopamine D1/D2 receptors revealed by experimental study and integrated in silico simulation. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 447-459.	2.9	6
129	A multiple-step <i>in silico</i> screening protocol to identify allosteric inhibitors of Spike-hACE2 binding. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4305-4316.	2.8	6
130	Drug-Drug Interaction Between Oxycodone and Diazepam by a Combined <i>In Silico</i> Pharmacokinetic and Pharmacodynamic Modeling Approach. <i>ACS Chemical Neuroscience</i> , 2021, 12, 1777-1790.	3.5	5
131	Molecular Mechanism of Ultrasound-Induced Structural Defects in Liposomes: A Nonequilibrium Molecular Dynamics Simulation Study. <i>Langmuir</i> , 2021, 37, 7945-7954.	3.5	5
132	Nonequilibrium atomistic molecular dynamics simulation of tubular nanomotor propelled by bubble propulsion. <i>Journal of Chemical Physics</i> , 2019, 151, 024103.	3.0	4
133	In Silico Screen Identifies a New Family of Agonists for the Bacterial Mechanosensitive Channel MscL. <i>Antibiotics</i> , 2022, 11, 433.	3.7	4
134	RNPS1 inhibits excessive tumor necrosis factor/tumor necrosis factor receptor signaling to support hematopoiesis in mice. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2200128119.	7.1	4
135	Challenges in Binding Free Energy Calculation using MM-PB/GBSA. <i>Bioenergetics: Open Access</i> , 2012, 01, .	0.1	3
136	Nonequilibrium molecular dynamics simulations of infrared laser-induced dissociation of a tetrameric A β 242 β -barrel in a neuronal membrane model. <i>Chemistry and Physics of Lipids</i> , 2021, 234, 105030.	3.2	2
137	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. , 2000, 21, 1049.		2
138	Development and Evaluation of Geometry Optimization Algorithms in Conjunction with ANI Potentials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 978-991.	5.3	2
139	Joint Computational/Cell-Based Approach for Screening Inhibitors of Tau Oligomerization: A Proof-of-Concept Study. <i>Journal of Alzheimer's Disease</i> , 2022, 89, 107-119.	2.6	2
140	Molecular Dynamics Simulations of a Protein Crystal. <i>Bioenergetics: Open Access</i> , 2014, 02, .	0.1	1
141	Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. <i>Journal of Cheminformatics</i> , 2021, 13, 11.	6.1	1
142	Structure and dynamics of major histocompatibility class Ib molecule H2-M3 complexed with mitochondrial-derived peptides. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 10300-10312.	3.5	1
143	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. , 0, .		1
144	In Silico Prediction of Pharmacokinetic Profile for Human Oral Drug Candidates Which Lack Clinical Pharmacokinetic Experiment Data. <i>European Journal of Drug Metabolism and Pharmacokinetics</i> , 2022, , 1.	1.6	1

#	ARTICLE	IF	CITATIONS
145	Physiologically-Based Pharmacokinetics Modeling for Hydroxychloroquine as a Treatment for Malaria and Optimized Dosing Regimens for Different Populations. <i>Journal of Personalized Medicine</i> , 2022, 12, 796.	2.5	1
146	Correction to Application of Molecular Dynamics Simulations in Molecular Property Prediction. 1. Density and Heat of Vaporization. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2333-2333.	5.3	0
147	MORT: a powerful foundational library for computational biology and CADD. <i>Journal of Cheminformatics</i> , 2014, 6, .	6.1	0