Jing Huang

List of Publications by Year in descending order

80 papers	9,538 citations	218381 26 h-index	71532 76 g-index
91 all docs	91 docs citations	91 times ranked	12194 citing authors

#	Article	IF	Citations
1	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. Nature Methods, 2017, 14, 71-73.	9.0	3,959
2	CHARMM36 all-atom additive protein force field: Validation based on comparison to NMR data. Journal of Computational Chemistry, 2013, 34, 2135-2145.	1.5	2,613
3	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. Chemical Reviews, 2016, 116, 4983-5013.	23.0	434
4	AXL is a candidate receptor for SARS-CoV-2 that promotes infection of pulmonary and bronchial epithelial cells. Cell Research, 2021, 31, 126-140.	5.7	356
5	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2013, 9, 5430-5449.	2.3	329
6	Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model. Journal of Physical Chemistry Letters, 2014, 5, 3144-3150.	2.1	139
7	Force field development and simulations of intrinsically disordered proteins. Current Opinion in Structural Biology, 2018, 48, 40-48.	2.6	139
8	Characterization, antioxidant and immunomodulatory effects of selenized polysaccharides from dandelion roots. Carbohydrate Polymers, 2021, 260, 117796.	5.1	78
9	Molecular dynamics simulations using the drude polarizable force field on GPUs with OpenMM: Implementation, validation, and benchmarks. Journal of Computational Chemistry, 2018, 39, 1682-1689.	1.5	77
10	Induction of Peptide Bond Dipoles Drives Cooperative Helix Formation in the (AAQAA)3 Peptide. Biophysical Journal, 2014, 107, 991-997.	0.2	76
11	CHARMM36: An Improved Force Field for Folded and Intrinsically Disordered Proteins. Biophysical Journal, 2017, 112, 175a-176a.	0.2	56
12	Machine-Learning-Assisted Free Energy Simulation of Solution-Phase and Enzyme Reactions. Journal of Chemical Theory and Computation, 2021, 17, 5745-5758.	2.3	55
13	Nanocrystals for improved dermal drug delivery. European Journal of Pharmaceutics and Biopharmaceutics, 2018, 128, 170-178.	2.0	54
14	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. Journal of Chemical Theory and Computation, 2020, 16, 3221-3239.	2.3	53
15	Turning Defense into Offense: Defensin Mimetics as Novel Antibiotics Targeting Lipid II. PLoS Pathogens, 2013, 9, e1003732.	2.1	50
16	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. Journal of Chemical Theory and Computation, 2018, 14, 948-958.	2.3	50
17	Ligand Self-Assembling through Complementary Hydrogen-Bonding in the Coordination Sphere of a Transition Metal Center: The 6-Diphenylphosphanylpyridin-2(1H)-one System. Journal of the American Chemical Society, 2011, 133, 964-975.	6.6	44
18	Infrared and Near-Infrared Spectroscopy of Acetylacetone and Hexafluoroacetylacetone. Journal of Physical Chemistry A, 2015, 119, 7980-7990.	1.1	43

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19	Structural insights into the gating mechanism of human SLC26A9 mediated by its C-terminal sequence. Cell Discovery, 2020, 6, 55.	3.1	43
20	Scan and Unlock: A Programmable DNA Molecular Automaton for Cellâ€Selective Activation of Ligandâ€Based Signaling. Angewandte Chemie - International Edition, 2021, 60, 6733-6743.	7.2	43
21	Mapping the Drude polarizable force field onto a multipole and induced dipole model. Journal of Chemical Physics, 2017, 147, 161702.	1.2	42
22	Kinetic isotope effect in malonaldehyde determined from path integral Monte Carlo simulations. Physical Chemistry Chemical Physics, 2014, 16, 204-211.	1.3	35
23	Enhanced Conformational Sampling Using Replica Exchange with Concurrent Solute Scaling and Hamiltonian Biasing Realized in One Dimension. Journal of Chemical Theory and Computation, 2015, 11, 2855-2867.	2.3	35
24	Conformational Heterogeneity of the HIV Envelope Glycan Shield. Scientific Reports, 2017, 7, 4435.	1.6	32
25	Induced Dipoleâ€“Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid Î²-Peptides. Journal of Physical Chemistry B, 2015, 119, 15574-15582.	1.2	30
26	TFPI is a colonic crypt receptor for TcdB from hypervirulent clade 2 C.Âdifficile. Cell, 2022, 185, 980-994.e15.	13.5	30
27	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. Molecules, 2018, 23, 2695.	1.7	29
28	Design, synthesis and bioevaluation of novel substituted triazines as potential dual PI3K/mTOR inhibitors. European Journal of Medicinal Chemistry, 2020, 204, 112637.	2.6	29
29	Distinct allosteric mechanisms of first-generation MsbA inhibitors. Science, 2021, 374, 580-585.	6.0	29
30	Screening active compounds from Corydalis yanhusuo by combining high expression VEGF receptor HEK293 cell membrane chromatography with HPLC - ESI - IT - TOF - MSn method. Journal of Pharmaceutical and Biomedical Analysis, 2017, 136, 134-139.	1.4	27
31	Cryo-EM structure of the human heteromeric amino acid transporter b ^{0,+} AT-rBAT. Science Advances, 2020, 6, eaay6379.	4.7	27
32	Cell membrane chromatography coupled with UHPLCâ€“ESIâ€“MS/MS method to screen target components from Peucedanum praeruptorum Dunn acting on Î±1A adrenergic receptor. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2016, 1011, 158-162.	1.2	25
33	An explicit-solvent hybrid QM and MM approach for predicting pKa of small molecules in SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1191-1201.	1.3	25
34	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. Journal of Chemical Theory and Computation, 2019, 15, 3854-3867.	2.3	25
35	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 989-1006.	1.3	24
36	<scp>CHARMMâ€GUI</scp> Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. Journal of Computational Chemistry, 2022, 43, 359-375.	1.5	24

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37	The inhibitory effect of piperine from Fructus piperis extract on the degranulation of RBL-2H3 cells. FÃ¬toterapÃ¬Ã¢, 2014, 99, 218-226.	1.1	20
38	Ardisimamillosides G and H, Two New Triterpenoid Saponins from Ardisia mamillata. Chemical and Pharmaceutical Bulletin, 2003, 51, 875-877.	0.6	19
39	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. Journal of Chemical Theory and Computation, 2017, 13, 679-695.	2.3	19
40	Structure of Penta-Alanine Investigated by Two-Dimensional Infrared Spectroscopy and Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2016, 120, 5325-5339.	1.2	18
41	Glucagon-like peptide-1 cleavage product GLP-1(9â€“36) reduces neuroinflammation from stroke via the activation of insulin-like growth factor 1 receptor in astrocytes. European Journal of Pharmacology, 2020, 887, 173581.	1.7	18
42	Scan and Unlock: A Programmable DNA Molecular Automaton for Cellâ€Selective Activation of Ligandâ€Based Signaling. Angewandte Chemie, 2021, 133, 6807-6817.	1.6	17
43	Explicit Hydrogen-Bond Potentials and Their Application to NMR Scalar Couplings in Proteins. Journal of Chemical Theory and Computation, 2010, 6, 467-476.	2.3	16
44	Hydrogen-Bond and Solvent Dynamics in Transition Metal Complexes: A Combined Simulation and NMR-Investigation. Journal of Physical Chemistry B, 2012, 116, 14406-14415.	1.2	16
45	Inhibitory effect of atenolol on urinary excretion of metformin via down-regulating multidrug and toxin extrusion protein 1 (rMate1) expression in the kidney of rats. European Journal of Pharmaceutical Sciences, 2015, 68, 18-26.	1.9	16
46	Absolute binding free energies for octa-acids and guests in SAMPL5. Journal of Computer-Aided Molecular Design, 2017, 31, 107-118.	1.3	16
47	Influence of Shenxiong Glucose Injection on the Activities of Six CYP Isozymes and Metabolism of Warfarin in Rats Assessed Using Probe Cocktail and Pharmacokinetic Approaches. Molecules, 2017, 22, 1994.	1.7	15
48	<scp>DIRECTâ€D</scp>: An automated method to identify and quantify conformational variationsâ€”application to Î²₂â€adrenergic <scp>GPCR</scp>. Journal of Computational Chemistry, 2016, 37, 416-425.	1.5	13
49	Absolute binding free energy calculations of CBClip hostâ€“guest systems in the SAMPL5 blind challenge. Journal of Computer-Aided Molecular Design, 2017, 31, 71-85.	1.3	13
50	Rational exploration of fold atlas for human solute carrier proteins. Structure, 2022, 30, 1321-1330.e5.	1.6	13
51	Characterization of Compounds Acting on the Î±1A Adrenergic Receptor fromCaulis spatholobiby Cell Membrane Chromatography with Possible Application for Treatment of Benign Prostatic Hyperplasia. Analytical Letters, 2014, 47, 1661-1669.	1.0	11
52	Comparison of the pharmacokinetic profiles of 13 phenolic acids and 6 triterpenes in normal and leukopenia rats after oral administration of Sanguisorba officinalis L. extract by LCâ€MS/MS. Journal of Separation Science, 2020, 43, 4103-4122.	1.3	11
53	Dynamical potential approach to DCO highly excited vibration. Chemical Physics Letters, 2007, 439, 231-235.	1.2	9
54	Pharmacokinetic herb-drug interactions between Aidi injection and doxorubicin in rats with diethylnitrosamine-induced hepatocellular carcinoma. BMC Pharmacology & Toxicology, 2021, 22, 48.	1.0	9

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55	Conformational Heterogeneity of Intracellular Loop 3 of the Î¼-opioid G-protein Coupled Receptor. Journal of Physical Chemistry B, 2016, 120, 11897-11904.	1.2	8
56	Survival-Associated Alternative Splicing Events in Pan-Renal Cell Carcinoma. Frontiers in Oncology, 2019, 9, 1317.	1.3	8
57	Discovery of the First Examples of Threonine Tyrosine Kinase PROTAC Degraders. Journal of Medicinal Chemistry, 2022, 65, 2313-2328.	2.9	8
58	Structure–activity exploration of a small-molecule Lipid II inhibitor. Drug Design, Development and Therapy, 2015, 9, 2383.	2.0	7
59	Towards Development of Small Molecule Lipid II Inhibitors as Novel Antibiotics. PLoS ONE, 2016, 11, e0164515.	1.1	7
60	Binding Energy and Free Energy of Calcium Ion to Calmodulin EF-Hands with the Drude Polarizable Force Field. ACS Physical Chemistry Au, 2022, 2, 143-155.	1.9	7
61	Predicting partition coefficients of drug-like molecules in the SAMPL6 challenge with Drude polarizable force fields. Journal of Computer-Aided Molecular Design, 2020, 34, 421-435.	1.3	6
62	Determination of Triterpenoids and Phenolic Acids from Sanguisorba officinalis L. by HPLC-ELSD and Its Application. Molecules, 2021, 26, 4505.	1.7	6
63	Design, Synthesis, and Biological Evaluation of 2-Formyl Tetrahydronaphthyridine Urea Derivatives as New Selective Covalently Reversible FGFR4 Inhibitors. Journal of Medicinal Chemistry, 2022, 65, 3249-3265.	2.9	6
64	Force field refinement from NMR scalar couplings. Chemical Physics, 2012, 396, 116-123.	0.9	5
65	Validating the CHARMM36m protein force field with LJ-PME reveals altered hydrogen bonding dynamics under elevated pressures. Communications Chemistry, 2021, 4, .	2.0	5
66	Atomistic simulations of reactive processes in the gas- and condensed-phase. International Reviews in Physical Chemistry, 2012, 31, 235-264.	0.9	4
67	Differential changes in the pharmacokinetics of doxorubicin in diethylnitrosamine-induced hepatocarcinoma model rats. Xenobiotica, 2020, 50, 1251-1257.	0.5	4
68	Characterization and Biological Activities of Polysaccharides from Dandelion (<i>Taraxacum) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 222 T	1.1	4
69	Methylguanidinium at the Air/Water Interface: A Simulation Study with the Drude Polarizable Force Field. Journal of Physical Chemistry B, 2021, 125, 393-405.	1.2	4
70	EViS: An Enhanced Virtual Screening Approach Based on Pocketâ€“Ligand Similarity. Journal of Chemical Information and Modeling, 2022, 62, 498-510.	2.5	4
71	Cooperative Helix Formation in the (AAQAA)3 Peptide Obtained with the Drude Polarizable Force Field. Biophysical Journal, 2015, 108, 518a.	0.2	3
72	Interactions Between Nucleosomes: From Atomistic Simulation to Polymer Model. Frontiers in Molecular Biosciences, 2021, 8, 624679.	1.6	3

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73	Proteinâ€“Ligand Binding Molecular Details Revealed by Terahertz Optical Kerr Spectroscopy: A Simulation Study. Jacs Au, 2021, 1, 1788-1797.	3.6	3
74	Pharmacokinetics, Tissue Distribution, and Excretion Study of Cajanonic Acid A in Rats by UPLC-MS/MS. Planta Medica, 2020, 86, 312-318.	0.7	2
75	Enhanced Conformational Sampling of Carbohydrates using Biasing Potential and Solute Tempering Replica Exchange: Application to the N-glycan on the HIV gp120 Envelope Protein. Biophysical Journal, 2015, 108, 157a.	0.2	1
76	Wideâ€ranging analysis of survivalâ€related alternative splicing events in invasive breast carcinoma. Oncology Letters, 2020, 20, 1866-1878.	0.8	1
77	Identification of U937JAK3-M511I Acute Myeloid Leukemia Cells as a Sensitive Model to JAK3 Inhibitor. Frontiers in Oncology, 2021, 11, 807200.	1.3	1
78	Development of a Polarizable Force Field for Macromolecules Based on the Classical Drude Oscillator. Biophysical Journal, 2014, 106, 43a.	0.2	0
79	Capturing the Cooperativity of Backbone Hydrogen Bonding with Polarizable Force Fields. Biophysical Journal, 2019, 116, 143a.	0.2	0
80	Editorial: Special Issue on Polarizable Force Fields for Biomolecular Modelling. Journal of Computational Biophysics and Chemistry, 2022, 21, 389-390.	1.0	0