Jing Huang

List of Publications by Year in Descending Order

69 papers	5,192 citations	22 h-index	72 g-index
91 ext. papers	7,503 ext. citations	7.2 avg, IF	6.28 L-index

#	Paper	IF	Citations
69	TFPI is a colonic crypt receptor for TcdB from hypervirulent clade 2 C. difficile.. *Cell*, **2022**, 185, 980-994.e15	5.62	2
68	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
67	Identification of U937 Acute Myeloid Leukemia Cells as a Sensitive Model to JAK3 Inhibitor.. *Frontiers in Oncology*, **2021**, 11, 807200	5.3	0
66	Methylguanidinium at the Air/Water Interface: A Simulation Study with the Drude Polarizable Force Field. *Journal of Physical Chemistry B*, **2021**, 125, 393-405	3.4	3
65	Interactions Between Nucleosomes: From Atomistic Simulation to Polymer Model. *Frontiers in Molecular Biosciences*, **2021**, 8, 624679	5.6	0
64	Characterization, antioxidant and immunomodulatory effects of selenized polysaccharides from dandelion roots. *Carbohydrate Polymers*, **2021**, 260, 117796	10.3	21
63	Scan and Unlock: A Programmable DNA Molecular Automaton for Cell-Selective Activation of Ligand-Based Signaling. *Angewandte Chemie - International Edition*, **2021**, 60, 6733-6743	16.4	13
62	Scan and Unlock: A Programmable DNA Molecular Automaton for Cell-Selective Activation of Ligand-Based Signaling. *Angewandte Chemie*, **2021**, 133, 6807-6817	3.6	5
61	Characterization and Biological Activities of Polysaccharides from Dandelion (Taraxacum officinale) Leaves. *Starch/Staerke*, **2021**, 73, 2000051	2.3	1
60	Distinct allosteric mechanisms of first-generation MsbA inhibitors. *Science*, **2021**, 374, 580-585	33.3	5
59	Machine-Learning-Assisted Free Energy Simulation of Solution-Phase and Enzyme Reactions. *Journal of Chemical Theory and Computation*, **2021**, 17, 5745-5758	6.4	14
58	Protein-Ligand Binding Molecular Details Revealed by Terahertz Optical Kerr Spectroscopy: A Simulation Study. *Jacs Au*, **2021**, 1, 1788-1797		1
57	Pharmacokinetic herb-drug interactions between Aidi injection and doxorubicin in rats with diethylnitrosamine-induced hepatocellular carcinoma. *BMC Pharmacology & Toxicology*, **2021**, 22, 48	2.6	1
56	AXL is a candidate receptor for SARS-CoV-2 that promotes infection of pulmonary and bronchial epithelial cells. *Cell Research*, **2021**, 31, 126-140	24.7	165
55	CHARMM-GUI Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. *Journal of Computational Chemistry*, **2021**,	3.5	4
54	Differential changes in the pharmacokinetics of doxorubicin in diethylnitrosamine-induced hepatocarcinoma model rats. *Xenobiotica*, **2020**, 50, 1251-1257	2	4
53	Pharmacokinetics, Tissue Distribution, and Excretion Study of Cajanonic Acid A in Rats by UPLC-MS/MS. *Planta Medica*, **2020**, 86, 312-318	3.1	1

52	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	4.2	4
51	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. *Journal of Chemical Theory and Computation*, **2020**, 16, 3221-3239	6.4	22
50	Wide-ranging analysis of survival-related alternative splicing events in invasive breast carcinoma. *Oncology Letters*, **2020**, 20, 1866-1878	2.6	1
49	Design, synthesis and bioevaluation of novel substituted triazines as potential dual PI3K/mTOR inhibitors. *European Journal of Medicinal Chemistry*, **2020**, 204, 112637	6.8	11
48	Glucagon-like peptide-1 cleavage product GLP-1(9-36) reduces neuroinflammation from stroke via the activation of insulin-like growth factor 1 receptor in astrocytes. *European Journal of Pharmacology*, **2020**, 887, 173581	5.3	5
47	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 LC-MS/MS. *Journal of Separation Science*, **2020**, 43, 4103-4122	3.4	5
46	Structural insights into the gating mechanism of human SLC26A9 mediated by its C-terminal sequence. *Cell Discovery*, **2020**, 6, 55	22.3	14
45	Cryo-EM structure of the human heteromeric amino acid transporter bAT-rBAT. *Science Advances*, **2020**, 6, eaay6379	14.3	13
44	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. *Journal of Chemical Theory and Computation*, **2019**, 15, 3854-3867	6.4	19
43	Survival-Associated Alternative Splicing Events in Pan-Renal Cell Carcinoma. *Frontiers in Oncology*, **2019**, 9, 1317	5.3	2
42	Nanocrystals for improved dermal drug delivery. *European Journal of Pharmaceutics and Biopharmaceutics*, **2018**, 128, 170-178	5.7	36
41	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	6.4	31
40	Force field development and simulations of intrinsically disordered proteins. *Current Opinion in Structural Biology*, **2018**, 48, 40-48	8.1	98
39	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	4.2	15
38	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. *Molecules*, **2018**, 23,	4.8	23
37	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	3.5	24
36	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	6.4	14
35	CHARMM36: An Improved Force Field for Folded and Intrinsically Disordered Proteins. *Biophysical Journal*, **2017**, 112, 175a-176a	2.9	33

34	Absolute binding free energies for octa-acids and guests in SAMPL5 : Evaluating binding free energies for octa-acid and guest complexes in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 107-118	4.2	15
33	Mapping the Drude polarizable force field onto a multipole and induced dipole model. *Journal of Chemical Physics*, **2017**, 147, 161702	3.9	32
32	Conformational Heterogeneity of the HIV Envelope Glycan Shield. *Scientific Reports*, **2017**, 7, 4435	4.9	22
31	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. *Nature Methods*, **2017**, 14, 71-73	21.6	1819
30	Absolute binding free energy calculations of CBClip host-guest systems in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 71-85	4.2	9
29	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,	4.8	9
28	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	4.2	20
27	Conformational Heterogeneity of Intracellular Loop 3 of the □opioid G-protein Coupled Receptor. *Journal of Physical Chemistry B*, **2016**, 120, 11897-11904	3.4	8
26	Cell membrane chromatography coupled with UHPLC-ESI-MS/MS method to screen target components from Peucedanum praeruptorum Dunn acting on □A adrenergic receptor. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2016**, 1011, 158-62	3.2	21
25	Structure of Penta-Alanine Investigated by Two-Dimensional Infrared Spectroscopy and Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 5325-39	3.4	13
24	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. *Chemical Reviews*, **2016**, 116, 4983-5013	68.1	299
23	Towards Development of Small Molecule Lipid II Inhibitors as Novel Antibiotics. *PLoS ONE*, **2016**, 11, e0164515	3.7	7
22	DIRECT-ID: An automated method to identify and quantify conformational variations--application to □ -adrenergic GPCR. *Journal of Computational Chemistry*, **2016**, 37, 416-25	3.5	12
21	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, 2855-67	6.4	25
20	Infrared and Near-Infrared Spectroscopy of Acetylacetone and Hexafluoroacetylacetone. *Journal of Physical Chemistry A*, **2015**, 119, 7980-90	2.8	32
19	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	5.1	13
18	Structure-activity exploration of a small-molecule Lipid II inhibitor. *Drug Design, Development and Therapy*, **2015**, 9, 2383-94	4.4	6
17	Induced Dipole-Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid □Peptides. *Journal of Physical Chemistry B*, **2015**, 119, 15574-82	3.4	23

16	Kinetic isotope effect in malonaldehyde determined from path integral Monte Carlo simulations. *Physical Chemistry Chemical Physics*, **2014**, 16, 204-11	3.6	30
15	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	6.4	111
14	Induction of peptide bond dipoles drives cooperative helix formation in the (AAQAA)3 peptide. *Biophysical Journal*, **2014**, 107, 991-7	2.9	60
13	The inhibitory effect of piperine from Fructus piperis extract on the degranulation of RBL-2H3 cells. *Fitoterapia*, **2014**, 99, 218-26	3.2	20
12	Characterization of Compounds Acting on the α1A Adrenergic Receptor from Caulis spatholobi by Cell Membrane Chromatography with Possible Application for Treatment of Benign Prostatic Hyperplasia. *Analytical Letters*, **2014**, 47, 1661-1669	2.2	10
11	CHARMM36 all-atom additive protein force field: validation based on comparison to NMR data. *Journal of Computational Chemistry*, **2013**, 34, 2135-45	3.5	1487
10	Force Field for Peptides and Proteins based on the Classical Drude Oscillator. *Journal of Chemical Theory and Computation*, **2013**, 9, 5430-5449	6.4	274
9	Force Field Treatment of Proton and Hydrogen Transfer in Molecular Systems **2013**, 253-276		1
8	Turning defense into offense: defensin mimetics as novel antibiotics targeting lipid II. *PLoS Pathogens*, **2013**, 9, e1003732	7.6	41
7	Hydrogen-bond and solvent dynamics in transition metal complexes: a combined simulation and NMR-investigation. *Journal of Physical Chemistry B*, **2012**, 116, 14406-15	3.4	16
6	Atomistic simulations of reactive processes in the gas- and condensed-phase. *International Reviews in Physical Chemistry*, **2012**, 31, 235-264	7	3
5	Force field refinement from NMR scalar couplings. *Chemical Physics*, **2012**, 396, 116-123	2.3	5
4	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, 964-75	16.4	41
3	Explicit Hydrogen-Bond Potentials and Their Application to NMR Scalar Couplings in Proteins. *Journal of Chemical Theory and Computation*, **2010**, 6, 467-76	6.4	13
2	Dynamical potential approach to DCO highly excited vibration. *Chemical Physics Letters*, **2007**, 439, 231-235	2.3	7
1	Ardisimamillosides G and H, two new triterpenoid saponins from Ardisia mamillata. *Chemical and Pharmaceutical Bulletin*, **2003**, 51, 875-7	1.9	16