Ting-Jun Hou

List of Publications by Citations

354 papers	15,832 citations	64 h-index	111 g-index
383 ext. papers	19,505 ext. citations	6.9 avg, IF	7.01 L-index

#	Paper	IF	Citations
354	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
353	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
352	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
351	Assessing the performance of MM/PBSA and MM/GBSA methods. 4. Accuracies of MM/PBSA and MM/GBSA methodologies evaluated by various simulation protocols using PDBbind data set. *Physical Chemistry Chemical Physics*, **2014**, 16, 16719-29	3.6	426
350	Comprehensive evaluation of ten docking programs on a diverse set of protein-ligand complexes: the prediction accuracy of sampling power and scoring power. *Physical Chemistry Chemical Physics*, **2016**, 18, 12964-75	3.6	400
349	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
348	Assessing the performance of MM/PBSA and MM/GBSA methods. 5. Improved docking performance using high solute dielectric constant MM/GBSA and MM/PBSA rescoring. *Physical Chemistry Chemical Physics*, **2014**, 16, 22035-45	3.6	322
347	Assessing the performance of the MM/PBSA and MM/GBSA methods. 6. Capability to predict protein-protein binding free energies and re-rank binding poses generated by protein-protein docking. *Physical Chemistry Chemical Physics*, **2016**, 18, 22129-39	3.6	246
346	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
345	Molecular dynamics and free energy studies on the wild-type and double mutant HIV-1 protease complexed with amprenavir and two amprenavir-related inhibitors: mechanism for binding and drug resistance. *Journal of Medicinal Chemistry*, **2007**, 50, 1177-88	8.3	216
344	The application of in silico drug-likeness predictions in pharmaceutical research. *Advanced Drug Delivery Reviews*, **2015**, 86, 2-10	18.5	190
343	Characterization of domain-peptide interaction interface: a case study on the amphiphysin-1 SH3 domain. *Journal of Molecular Biology*, **2008**, 376, 1201-14	6.5	179
342	ADME evaluation in drug discovery. 4. Prediction of aqueous solubility based on atom contribution approach. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 266-75		176
341	Characterization of domain-peptide interaction interface: prediction of SH3 domain-mediated protein-protein interaction network in yeast by generic structure-based models. *Journal of Proteome Research*, **2012**, 11, 2982-95	5.6	173
340	Janus Structures of Transition Metal Dichalcogenides as the Heterojunction Photocatalysts for Water Splitting. *Journal of Physical Chemistry C*, **2018**, 122, 3123-3129	3.8	160
339	Recent development and application of virtual screening in drug discovery: an overview. *Current Pharmaceutical Design*, **2004**, 10, 1011-33	3.3	158
338	Assessing the performance of MM/PBSA and MM/GBSA methods. 7. Entropy effects on the performance of end-point binding free energy calculation approaches. *Physical Chemistry Chemical Physics*, **2018**, 20, 14450-14460	3.6	149

337	ADMETlab 2.0: an integrated online platform for accurate and comprehensive predictions of ADMET properties. *Nucleic Acids Research*, **2021**, 49, W5-W14	20.1	148
336	Recent advances in computational prediction of drug absorption and permeability in drug discovery. *Current Medicinal Chemistry*, **2006**, 13, 2653-67	4.3	147
335	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
334	HawkDock: a web server to predict and analyze the protein-protein complex based on computational docking and MM/GBSA. *Nucleic Acids Research*, **2019**, 47, W322-W330	20.1	139
333	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
332	Computational analysis and prediction of the binding motif and protein interacting partners of the Abl SH3 domain. *PLoS Computational Biology*, **2006**, 2, e1	5	129
331	ADME evaluation in drug discovery. 5. Correlation of Caco-2 permeation with simple molecular properties. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1585-600		129
330	ADME evaluation in drug discovery. 10. Predictions of P-glycoprotein inhibitors using recursive partitioning and naive Bayesian classification techniques. *Molecular Pharmaceutics*, **2011**, 8, 889-900	5.6	125
329	Allosite: a method for predicting allosteric sites. *Bioinformatics*, **2013**, 29, 2357-9	7.2	117
328	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
327	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
326	Computational models for predicting substrates or inhibitors of P-glycoprotein. *Drug Discovery Today*, **2012**, 17, 343-51	8.8	107
325	Evaluating the potency of HIV-1 protease drugs to combat resistance. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1163-74	4.2	103
324	Potential Application of Novel Boron-Doped Graphene Nanoribbon as Oxygen Reduction Reaction Catalyst. *Journal of Physical Chemistry C*, **2016**, 120, 17427-17434	3.8	101
323	ADME evaluation in drug discovery. 3. Modeling blood-brain barrier partitioning using simple molecular descriptors. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 2137-52		98
322	Atomistic Origins of Surface Defects in CHNHPbBr Perovskite and Their Electronic Structures. *ACS Nano*, **2017**, 11, 2060-2065	16.7	93
321	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
320	Characterization of domain-peptide interaction interface: a generic structure-based model to decipher the binding specificity of SH3 domains. *Molecular and Cellular Proteomics*, **2009**, 8, 639-49	7.6	92

319	Structure-ADME relationship: still a long way to go?. *Expert Opinion on Drug Metabolism and Toxicology*, **2008**, 4, 759-70	5.5	92
318	Application of molecular dynamics simulations in molecular property prediction II: diffusion coefficient. *Journal of Computational Chemistry*, **2011**, 32, 3505-19	3.5	91
317	Drug-likeness analysis of traditional Chinese medicines: prediction of drug-likeness using machine learning approaches. *Molecular Pharmaceutics*, **2012**, 9, 2875-86	5.6	88
316	ADME evaluation in drug discovery. 1. Applications of genetic algorithms to the prediction of blood-brain partitioning of a large set of drugs. *Journal of Molecular Modeling*, **2002**, 8, 337-49	2	87
315	Two-dimensional germanium monochalcogenide photocatalyst for water splitting under ultraviolet, visible to near-infrared light. *Nanoscale*, **2017**, 9, 8608-8615	7.7	85
314	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
313	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
312	Recent advances on aqueous solubility prediction. *Combinatorial Chemistry and High Throughput Screening*, **2011**, 14, 328-38	1.3	83
311	Drug and drug candidate building block analysis. *Journal of Chemical Information and Modeling*, **2010**, 50, 55-67	6.1	83
310	Assessing an ensemble docking-based virtual screening strategy for kinase targets by considering protein flexibility. *Journal of Chemical Information and Modeling*, **2014**, 54, 2664-79	6.1	79
309	Mechanism of graphene oxide as an enzyme inhibitor from molecular dynamics simulations. *ACS Applied Materials & Interfaces*, **2014**, 6, 7153-63	9.5	79
308	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
307	MORT: a powerful foundational library for computational biology and CADD. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
306	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
305	Predictions of Binding of a Diverse Set of Ligands to Gelatinase-A by a Combination of Molecular Dynamics and Continuum Solvent Models. *Journal of Physical Chemistry B*, **2002**, 106, 5527-5535	3.4	76
304	Insight into crizotinib resistance mechanisms caused by three mutations in ALK tyrosine kinase using free energy calculation approaches. *Journal of Chemical Information and Modeling*, **2013**, 53, 2376-89	6.1	75
303	Two-Dimensional MnO2 as a Better Cathode Material for Lithium Ion Batteries. *Journal of Physical Chemistry C*, **2015**, 119, 28783-28788	3.8	75
302	A 3D structure database of components from Chinese traditional medicinal herbs. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 481-9		75

301	Detecting and understanding combinatorial mutation patterns responsible for HIV drug resistance. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 1321-6	11.5	72
300	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
299	Current developments of macrophage migration inhibitory factor (MIF) inhibitors. *Drug Discovery Today*, **2013**, 18, 592-600	8.8	71
298	ADMET evaluation in drug discovery. 13. Development of in silico prediction models for P-glycoprotein substrates. *Molecular Pharmaceutics*, **2014**, 11, 716-26	5.6	70
297	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
296	New Ti-decorated B40 fullerene as a promising hydrogen storage material. *Scientific Reports*, **2015**, 5, 9952	4.9	67
295	ADMET evaluation in drug discovery: 15. Accurate prediction of rat oral acute toxicity using relevance vector machine and consensus modeling. *Journal of Cheminformatics*, **2016**, 8, 6	8.6	67
294	Mapping the binding site of a large set of quinazoline type EGF-R inhibitors using molecular field analyses and molecular docking studies. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 273-87		66
293	Prediction of binding affinities between the human amphiphysin-1 SH3 domain and its peptide ligands using homology modeling, molecular dynamics and molecular field analysis. *Journal of Proteome Research*, **2006**, 5, 32-43	5.6	65
292	From machine learning to deep learning: Advances in scoring functions for protein□gand docking. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1429	7.9	65
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289	Discovery of novel inhibitors targeting the macrophage migration inhibitory factor via structure-based virtual screening and bioassays. *Journal of Medicinal Chemistry*, **2014**, 57, 3737-45	8.3	61
288	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
287	B40 fullerene: An efficient material for CO2 capture, storage and separation. *Current Applied Physics*, **2015**, 15, 1084-1089	2.6	60
286	ADMET Evaluation in Drug Discovery. 16. Predicting hERG Blockers by Combining Multiple Pharmacophores and Machine Learning Approaches. *Molecular Pharmaceutics*, **2016**, 13, 2855-66	5.6	60
285	Revealing the favorable dissociation pathway of type II kinase inhibitors via enhanced sampling simulations and two-end-state calculations. *Scientific Reports*, **2015**, 5, 8457	4.9	59
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282	Recent developments in computational prediction of HERG blockage. *Current Topics in Medicinal Chemistry*, **2013**, 13, 1317-26	3	57
281	Advances in the development of Rho-associated protein kinase (ROCK) inhibitors. *Drug Discovery Today*, **2013**, 18, 1323-33	8.8	56
280	Theoretical studies on the susceptibility of oseltamivir against variants of 2009 A/H1N1 influenza neuraminidase. *Journal of Chemical Information and Modeling*, **2012**, 52, 2715-29	6.1	56
279	Fast approaches for molecular polarizability calculations. *Journal of Physical Chemistry A*, **2007**, 111, 4443-8	2.8	56
278	SiC7 siligraphene: a novel donor material with extraordinary sunlight absorption. *Nanoscale*, **2016**, 8, 6994-9	7.7	54
277	Prediction of peptides binding to the PKA RIIalpha subunit using a hierarchical strategy. *Bioinformatics*, **2011**, 27, 1814-21	7.2	54
276	Development and evaluation of an integrated virtual screening strategy by combining molecular docking and pharmacophore searching based on multiple protein structures. *Journal of Chemical Information and Modeling*, **2013**, 53, 2743-56	6.1	53
275	Discovery and optimization of triazine derivatives as ROCK1 inhibitors: molecular docking, molecular dynamics simulations and free energy calculations. *Molecular BioSystems*, **2013**, 9, 361-74		53
274	Monolayer graphitic germanium carbide (g-GeC): the promising cathode catalyst for fuel cell and lithium–oxygen battery applications. *Journal of Materials Chemistry A*, **2018**, 6, 2212-2218	13	52
273	Heptazine-based graphitic carbon nitride as an effective hydrogen purification membrane. *RSC Advances*, **2016**, 6, 52377-52383	3.7	52
272	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
271	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
270	Theoretical investigations on SiC2 siligraphene as promising metal-free catalyst for oxygen reduction reaction. *Journal of Power Sources*, **2015**, 299, 371-379	8.9	50
269	Morphology and Performance of Polymer Solar Cell Characterized by DPD Simulation and Graph Theory. *Scientific Reports*, **2015**, 5, 16854	4.9	49
268	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
267	Theoretical investigations on novel SiC5 siligraphene as gas sensor for air pollutants. *Carbon*, **2017**, 113, 114-121	10.4	48
266	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

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262	Constructing and Validating High-Performance MIEC-SVM Models in Virtual Screening for Kinases: A Better Way for Actives Discovery. *Scientific Reports*, **2016**, 6, 24817	4.9	47
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260	Discovery of Rho-kinase inhibitors by docking-based virtual screening. *Molecular BioSystems*, **2013**, 9, 1511-21		46
259	Drug Discovery Targeting Anaplastic Lymphoma Kinase (ALK). *Journal of Medicinal Chemistry*, **2019**, 62, 10927-10954	8.3	44
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257	MoS2 supported single platinum atoms and their superior catalytic activity for CO oxidation: a density functional theory study. *Journal of Materials Chemistry A*, **2015**, 3, 23113-23119	13	43
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254	Computational modeling of structure-function of g protein-coupled receptors with applications for drug design. *Current Medicinal Chemistry*, **2010**, 17, 1167-80	4.3	42
253	Assessing the performance of the MM/PBSA and MM/GBSA methods. 10. Impacts of enhanced sampling and variable dielectric model on protein-protein Interactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 18958-18969	3.6	41
252	Importance of protein flexibility in ranking inhibitor affinities: modeling the binding mechanisms of piperidine carboxamides as Type I1/2 ALK inhibitors. *Physical Chemistry Chemical Physics*, **2015**, 17, 6098-113	3.6	41
251	Photophysical Studies on the Mono- and Dichromophoric Hemicyanine Dyes I. Photoelectric Conversion from the Dye Modified ITO Electrodes. *Journal of Physical Chemistry B*, **2002**, 106, 10020-10030	3.4	41
250	Farnesyltransferase and geranylgeranyltransferase I: structures, mechanism, inhibitors and molecular modeling. *Drug Discovery Today*, **2015**, 20, 267-76	8.8	40
249	ADMET Evaluation in Drug Discovery. 19. Reliable Prediction of Human Cytochrome P450 Inhibition Using Artificial Intelligence Approaches. *Journal of Chemical Information and Modeling*, **2019**, 59, 4587-4601	6.1	40
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245	Combined strategies in structure-based virtual screening. *Physical Chemistry Chemical Physics*, **2020**, 22, 3149-3159	3.6	39
244	PROTAC-DB: an online database of PROTACs. *Nucleic Acids Research*, **2021**, 49, D1381-D1387	20.1	39
243	Directly Binding Rather than Induced-Fit Dominated Binding Affinity Difference in (S)- and (R)-Crizotinib Bound MTH1. *Journal of Chemical Theory and Computation*, **2016**, 12, 851-60	6.4	38
242	Monolayer group IVA monochalcogenides as potential and efficient catalysts for the oxygen reduction reaction from first-principles calculations. *Journal of Materials Chemistry A*, **2017**, 5, 1734-1741	13	37
241	ADME evaluation in drug discovery. 2. Prediction of partition coefficient by atom-additive approach based on atom-weighted solvent accessible surface areas. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1058-67		37
240	Empirical Aqueous Solvation Models Based on Accessible Surface Areas with Implicit Electrostatics. *Journal of Physical Chemistry B*, **2002**, 106, 11295-11304	3.4	37
239	Structural basis of the interactions between CXCR4 and CXCL12/SDF-1 revealed by theoretical approaches. *Molecular BioSystems*, **2013**, 9, 2107-17		36
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232	Recent developments of in silico predictions of oral bioavailability. *Combinatorial Chemistry and High Throughput Screening*, **2011**, 14, 362-74	1.3	34
231	Could graph neural networks learn better molecular representation for drug discovery? A comparison study of descriptor-based and graph-based models. *Journal of Cheminformatics*, **2021**, 13, 12	8.6	34
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228	Improving the alkaline stability of imidazolium cations by substitution. *ChemPhysChem*, **2014**, 15, 3006-14	3.2	32
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209	The competitive binding between inhibitors and substrates of HCV NS3/4A protease: a general mechanism of drug resistance. *Antiviral Research*, **2014**, 103, 60-70	10.8	26
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206	Unraveling the allosteric inhibition mechanism of PTP1B by free energy calculation based on umbrella sampling. *Journal of Chemical Information and Modeling*, **2013**, 53, 1157-67	6.1	26
205	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
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203	Feasibility of using molecular docking-based virtual screening for searching dual target kinase inhibitors. *Journal of Chemical Information and Modeling*, **2013**, 53, 982-96	6.1	25
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