Ting-Jun Hou

List of Publications by Year in Descending Order

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	Discovery of a novel nonsteroidal selective glucocorticoid receptor modulator by virtual screening and bioassays.. *Acta Pharmacologica Sinica*, **2022**,	8	4
353	Knowledge-based BERT: a method to extract molecular features such as computational chemists.. *Briefings in Bioinformatics*, **2022**,	13.4	3
352	High-throughput glycolytic inhibitor discovery targeting glioblastoma by graphite dots-assisted LDI mass spectrometry.. *Science Advances*, **2022**, 8, eabl4923	14.3	0
351	The structure of erastin-bound xCT-4F2hc complex reveals molecular mechanisms underlying erastin-induced ferroptosis.. *Cell Research*, **2022**,	24.7	2
350	Characterizing the stabilization effects of stabilizers in protein-protein systems with end-point binding free energy calculations.. *Briefings in Bioinformatics*, **2022**,	13.4	3
349	Discovery of novel non-steroidal selective glucocorticoid receptor modulators by structure- and IGN-based virtual screening, structural optimization, and biological evaluation.. *European Journal of Medicinal Chemistry*, **2022**, 237, 114382	6.8	1
348	Machine learning to predict metabolic drug interactions related to cytochrome P450 isozymes.. *Journal of Cheminformatics*, **2022**, 14, 23	8.6	3
347	Do we need different machine learning algorithms for QSAR modeling? A comprehensive assessment of 16 machine learning algorithms on 14 QSAR data sets. *Briefings in Bioinformatics*, **2021**, 22,	13.4	18
346	Pterostilbene inhibits hepatocellular carcinoma proliferation and HBV replication by targeting ribonucleotide reductase M2 protein. *American Journal of Cancer Research*, **2021**, 11, 2975-2989	4.4	1
345	Deep learning approaches for de novo drug design: An overview. *Current Opinion in Structural Biology*, **2021**, 72, 135-144	8.1	5
344	Discovery of Novel GR Ligands toward Druggable GR Antagonist Conformations Identified by MD Simulations and Markov State Model Analysis. *Advanced Science*, **2021**, e2102435	13.6	6
343	A unified drug-target interaction prediction framework based on knowledge graph and recommendation system. *Nature Communications*, **2021**, 12, 6775	17.4	11
342	Semi-automated workflow for molecular pair analysis and QSAR-assisted transformation space expansion. *Journal of Cheminformatics*, **2021**, 13, 86	8.6	0
341	Discovery of a Novel Androgen Receptor Antagonist Manifesting Evidence to Disrupt the Dimerization of the Ligand-Binding Domain via Attenuating the Hydrogen-Bonding Network Between the Two Monomers. *Journal of Medicinal Chemistry*, **2021**, 64, 17221-17238	8.3	1
340	The impact of cross-docked poses on performance of machine learning classifier for protein-ligand binding pose prediction. *Journal of Cheminformatics*, **2021**, 13, 81	8.6	2
339	Discovery of novel DprE1 inhibitors via computational bioactivity fingerprints and structure-based virtual screening. *Acta Pharmacologica Sinica*, **2021**,	8	1
338	Multi-constraint molecular generation based on conditional transformer, knowledge distillation and reinforcement learning. *Nature Machine Intelligence*, **2021**, 3, 914-922	22.5	9

337	Integrative Modeling of PROTAC-Mediated Ternary Complexes. *Journal of Medicinal Chemistry*, **2021**, 64, 16271-16281	8.3	7
336	ChemFLuo: a web-server for structure analysis and identification of fluorescent compounds. *Briefings in Bioinformatics*, **2021**, 22,	13.4	3
335	Discovery of novel antagonists targeting the DNA binding domain of androgen receptor by integrated docking-based virtual screening and bioassays. *Acta Pharmacologica Sinica*, **2021**,	8	5
334	Hyperbolic relational graph convolution networks plus: a simple but highly efficient QSAR-modeling method. *Briefings in Bioinformatics*, **2021**, 22,	13.4	3
333	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
332	ARIH1 signaling promotes anti-tumor immunity by targeting PD-L1 for proteasomal degradation. *Nature Communications*, **2021**, 12, 2346	17.4	8
331	Identification of active molecules against Mycobacterium tuberculosis through machine learning. *Briefings in Bioinformatics*, **2021**, 22,	13.4	3
330	Discovery of novel HBV capsid assembly modulators by structure-based virtual screening and bioassays. *Bioorganic and Medicinal Chemistry*, **2021**, 36, 116096	3.4	2
329	Structural basis of GABA receptor-G protein coupling. *Nature*, **2021**, 594, 594-598	50.4	13
328	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	6.1	2
327	Computational Bioactivity Fingerprint Similarities To Navigate the Discovery of Novel Scaffolds. *Journal of Medicinal Chemistry*, **2021**, 64, 7544-7554	8.3	2
326	Mining Toxicity Information from Large Amounts of Toxicity Data. *Journal of Medicinal Chemistry*, **2021**, 64, 6924-6936	8.3	8
325	The MCR-3 inside linker appears as a facilitator of colistin resistance. *Cell Reports*, **2021**, 35, 109135	10.6	4
324	DeepChargePredictor: A web server for predicting QM-based atomic charges via state-of-the-art machine-learning algorithms. *Bioinformatics*, **2021**,	7.2	1
323	MG-BERT: leveraging unsupervised atomic representation learning for molecular property prediction. *Briefings in Bioinformatics*, **2021**, 22,	13.4	8
322	Benchmarking the mechanisms of frequent hitters: limitation of PAINS alerts. *Drug Discovery Today*, **2021**, 26, 1353-1358	8.8	9
321	Metformin activates chaperone-mediated autophagy and improves disease pathologies in an Alzheimer disease mouse model. *Protein and Cell*, **2021**, 12, 769-787	7.2	15
320	Discovery of a small molecule inhibitor of cullin neddylation that triggers ER stress to induce autophagy.. *Acta Pharmaceutica Sinica B*, **2021**, 11, 3567-3584	15.5	3

319	Regulation Mechanism for the Binding between the SARS-CoV-2 Spike Protein and Host Angiotensin-Converting Enzyme II. *Journal of Physical Chemistry Letters*, **2021**, 12, 6252-6261	6.4	3
318	Beware of the generic machine learning-based scoring functions in structure-based virtual screening. *Briefings in Bioinformatics*, **2021**, 22,	13.4	12
317	Improving structure-based virtual screening performance via learning from scoring function components. *Briefings in Bioinformatics*, **2021**, 22,	13.4	11
316	Can machine learning consistently improve the scoring power of classical scoring functions? Insights into the role of machine learning in scoring functions. *Briefings in Bioinformatics*, **2021**, 22, 497-514	13.4	23
315	PROTAC-DB: an online database of PROTACs. *Nucleic Acids Research*, **2021**, 49, D1381-D1387	20.1	39
314	CovalentInDB: a comprehensive database facilitating the discovery of covalent inhibitors. *Nucleic Acids Research*, **2021**, 49, D1122-D1129	20.1	14
313	Current advances in ligand-based target prediction. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1504	7.9	8
312	Targeting phosphatidylinositol 3-kinase gamma (PI3Kγ): Discovery and development of its selective inhibitors. *Medicinal Research Reviews*, **2021**, 41, 1599-1621	14.4	6
311	Scopy: an integrated negative design python library for desirable HTS/VS database design. *Briefings in Bioinformatics*, **2021**, 22,	13.4	6
310	DeepAtomicCharge: a new graph convolutional network-based architecture for accurate prediction of atomic charges. *Briefings in Bioinformatics*, **2021**, 22,	13.4	5
309	BioMedR: an R/CRAN package for integrated data analysis pipeline in biomedical study. *Briefings in Bioinformatics*, **2021**, 22, 474-484	13.4	3
308	Accuracy or novelty: what can we gain from target-specific machine-learning-based scoring functions in virtual screening?. *Briefings in Bioinformatics*, **2021**, 22,	13.4	6
307	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
306	ASFP (Artificial Intelligence based Scoring Function Platform): a web server for the development of customized scoring functions. *Journal of Cheminformatics*, **2021**, 13, 6	8.6	4
305	Discovery of novel MIF inhibitors that attenuate microglial inflammatory activation by structures-based virtual screening and in vitro bioassays. *Acta Pharmacologica Sinica*, **2021**,	8	1
304	Structural insights into ligand recognition and activation of the melanocortin-4 receptor. *Cell Research*, **2021**, 31, 1163-1175	24.7	2
303	Learning to SMILES: BAN-based strategies to improve latent representation learning from molecules. *Briefings in Bioinformatics*, **2021**, 22,	13.4	4
302	Discovery of a Novel Mitogen-Activated Protein Kinase (FgGpmk1) Inhibitor for the Treatment of Fusarium Head Blight. *Journal of Medicinal Chemistry*, **2021**, 64, 13841-13852	8.3	2

301	Opportunities for overcoming tuberculosis: Emerging targets and their inhibitors. *Drug Discovery Today*, **2021**, 27, 326-326	8.8	3
300	Inhibition of neuroinflammation by MIF inhibitor 3-({[4-(4-methoxyphenyl)-6-methyl-2-pyrimidinyl]thio}1methyl)benzoic acid (Z-312). *International Immunopharmacology*, **2021**, 98, 107868	5.8	1
299	Characterizing the Morphology and Efficiency of Organic Solar Cells by Multiscale Simulations. *Springer Series in Materials Science*, **2021**, 679-692	0.9	
298	QSAR-assisted-MMPA to expand chemical transformation space for lead optimization. *Briefings in Bioinformatics*, **2021**, 22,	13.4	3
297	DDInter: an online drug-drug interaction database towards improving clinical decision-making and patient safety. *Nucleic Acids Research*, **2021**,	20.1	6
296	InteractionGraphNet: A Novel and Efficient Deep Graph Representation Learning Framework for Accurate Protein-Ligand Interaction Predictions. *Journal of Medicinal Chemistry*, **2021**,	8.3	11
295	Fast and accurate prediction of partial charges using Atom-Path-Descriptor-based machine learning. *Bioinformatics*, **2020**, 36, 4721-4728	7.2	5
294	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	6.1	13
293	Gossypol inhibits cullin neddylation by targeting SAG-CUL5 and RBX1-CUL1 complexes. *Neoplasia*, **2020**, 22, 179-191	6.4	8
292	Structural Analysis and Identification of False Positive Hits in Luciferase-Based Assays. *Journal of Chemical Information and Modeling*, **2020**, 60, 2031-2043	6.1	8
291	ADMET evaluation in drug discovery. 20. Prediction of breast cancer resistance protein inhibition through machine learning. *Journal of Cheminformatics*, **2020**, 12, 16	8.6	20
290	Binding affinity and dissociation pathway predictions for a series of USP7 inhibitors with pyrimidinone scaffold by multiple computational methods. *Physical Chemistry Chemical Physics*, **2020**, 22, 5487-5499	3.6	4
289	Novel androgen receptor antagonist identified by structure-based virtual screening, structural optimization, and biological evaluation. *European Journal of Medicinal Chemistry*, **2020**, 192, 112156	6.8	7
288	Frequent hitters: nuisance artifacts in high-throughput screening. *Drug Discovery Today*, **2020**, 25, 657-667	8.8	23
287	Improving Docking-Based Virtual Screening Ability by Integrating Multiple Energy Auxiliary Terms from Molecular Docking Scoring. *Journal of Chemical Information and Modeling*, **2020**, 60, 4216-4230	6.1	17
286	Structure-based discovery of CZL80, a caspase-1 inhibitor with therapeutic potential for febrile seizures and later enhanced epileptogenic susceptibility. *British Journal of Pharmacology*, **2020**, 177, 3519-3534	8.6	7
285	Synthesis and biological evaluation of heterocyclic bis-aryl amides as novel Src homology 2 domain containing protein tyrosine phosphatase-2 (SHP2) inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2020**, 30, 127170	2.9	6
284	Advances in the computational development of androgen receptor antagonists. *Drug Discovery Today*, **2020**, 25, 1453-1461	8.8	11

283	Combined strategies in structure-based virtual screening. *Physical Chemistry Chemical Physics*, **2020**, 22, 3149-3159	3.6	39
282	Application of Negative Design To Design a More Desirable Virtual Screening Library. *Journal of Medicinal Chemistry*, **2020**, 63, 4411-4429	8.3	14
281	Systematic Modeling of log Based on Ensemble Machine Learning, Group Contribution, and Matched Molecular Pair Analysis. *Journal of Chemical Information and Modeling*, **2020**, 60, 63-76	6.1	20
280	Insight Derived from Molecular Dynamics Simulation into the Selectivity Mechanism Targeting G-Quadruplex. *Journal of Physical Chemistry B*, **2020**, 124, 9773-9784	3.4	4
279	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
278	Comprehensive Evaluation of Fourteen Docking Programs on Protein-Peptide Complexes. *Journal of Chemical Theory and Computation*, **2020**, 16, 3959-3969	6.4	32
277	Structural Analysis and Identification of Colloidal Aggregators in Drug Discovery. *Journal of Chemical Information and Modeling*, **2019**, 59, 3714-3726	6.1	23
276	Discovery of 3,6-diaryl-1H-pyrazolo[3,4-b]pyridines as potent anaplastic lymphoma kinase (ALK) inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2019**, 29, 912-916	2.9	9
275	Communication between the Ligand-Binding Pocket and the Activation Function-2 Domain of Androgen Receptor Revealed by Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 842-857	6.1	17
274	Voltage-gated sodium channels: structures, functions, and molecular modeling. *Drug Discovery Today*, **2019**, 24, 1389-1397	8.8	19
273	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
272	Insight into the selective binding mechanism of DNMT1 and DNMT3A inhibitors: a molecular simulation study. *Physical Chemistry Chemical Physics*, **2019**, 21, 12931-12947	3.6	23
271	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
270	Assessing the performance of MM/PBSA and MM/GBSA methods. 9. Prediction reliability of binding affinities and binding poses for protein-peptide complexes. *Physical Chemistry Chemical Physics*, **2019**, 21, 10135-10145	3.6	47
269	Increased gene copy number of worsens sepsis by inducing endothelial pyroptosis. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 3161-3170	11.5	24
268	The inflammatory cytokine IL-6 induces FRA1 deacetylation promoting colorectal cancer stem-like properties. *Oncogene*, **2019**, 38, 4932-4947	9.2	26
267	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
266	Drug Discovery Targeting Anaplastic Lymphoma Kinase (ALK). *Journal of Medicinal Chemistry*, **2019**, 62, 10927-10954	8.3	44

265	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
264	DNA methyltransferases: emerging targets for the discovery of inhibitors as potent anticancer drugs. *Drug Discovery Today*, **2019**, 24, 2323-2331	8.8	25
263	Importance of a crystalline water network in docking-based virtual screening: a case study of BRD4. *Physical Chemistry Chemical Physics*, **2019**, 21, 25276-25289	3.6	12
262	Identification of an Activating Mutation in the Extracellular Domain of HER2 Conferring Resistance to Pertuzumab. *OncoTargets and Therapy*, **2019**, 12, 11597-11608	4.4	4
261	A magic drug target: Androgen receptor. *Medicinal Research Reviews*, **2019**, 39, 1485-1514	14.4	17
260	farPPI: a webserver for accurate prediction of protein-ligand binding structures for small-molecule PPI inhibitors by MM/PB(GB)SA methods. *Bioinformatics*, **2019**, 35, 1777-1779	7.2	33
259	The adsorption, diffusion and capacity of lithium on novel boron-doped graphene nanoribbon: A density functional theory study. *Applied Surface Science*, **2019**, 466, 737-745	6.7	15
258	Reliability of Docking-Based Virtual Screening for GPCR Ligands with Homology Modeled Structures: A Case Study of the Angiotensin II Type I Receptor. *ACS Chemical Neuroscience*, **2019**, 10, 677-689	5.7	17
257	Fullerene derivatives act as inhibitors of leukocyte common antigen based on molecular dynamics simulations.. *RSC Advances*, **2018**, 8, 13997-14008	3.7	7
256	Macrophage migration inhibitory factor (MIF) inhibitor, Z-590 suppresses cartilage destruction in adjuvant-induced arthritis via inhibition of macrophage inflammatory activation. *Immunopharmacology and Immunotoxicology*, **2018**, 40, 149-157	3.2	7
255	Benchmark Study Based on 2P2I to Gain Insights into the Discovery of Small-Molecule PPI Inhibitors. *Journal of Physical Chemistry B*, **2018**, 122, 2544-2555	3.4	11
254	Importance of protein flexibility in molecular recognition: a case study on Type-I1/2 inhibitors of ALK. *Physical Chemistry Chemical Physics*, **2018**, 20, 4851-4863	3.6	21
253	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
252	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
251	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
250	Two-dimensional siligraphenes as cathode catalysts for nonaqueous lithium-oxygen batteries. *Carbon*, **2018**, 126, 580-587	10.4	31
249	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
248	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

247	Discovery of Novel Androgen Receptor Ligands by Structure-based Virtual Screening and Bioassays. *Genomics, Proteomics and Bioinformatics*, **2018**, 16, 416-427	6.5	19
246	Origin of the catalytic activity of phosphorus doped MoS for oxygen reduction reaction (ORR) in alkaline solution: a theoretical study. *Scientific Reports*, **2018**, 8, 13292	4.9	13
245	Comprehensive assessment of nine docking programs on type II kinase inhibitors: prediction accuracy of sampling power, scoring power and screening power. *Briefings in Bioinformatics*, **2018**,	13.4	8
244	Structure-Based Drug Design and Identification of HO-Soluble and Low Toxic Hexacyclic Camptothecin Derivatives with Improved Efficacy in Cancer and Lethal Inflammation Models in Vivo. *Journal of Medicinal Chemistry*, **2018**, 61, 8613-8624	8.3	19
243	Cheminformatic Insight into the Differences between Terrestrial and Marine Originated Natural Products. *Journal of Chemical Information and Modeling*, **2018**, 58, 1182-1193	6.1	32
242	Peptide-Tethered Hydrogel Scaffold Promotes Recovery from Spinal Cord Transection via Synergism with Mesenchymal Stem Cells. *ACS Applied Materials & Interfaces*, **2017**, 9, 3330-3342	9.5	61
241	Atomistic Origins of Surface Defects in CHNHPbBr Perovskite and Their Electronic Structures. *ACS Nano*, **2017**, 11, 2060-2065	16.7	93
240	Discovery of Novel and Selective Adenosine A Receptor Antagonists for Treating Parkinson's Disease through Comparative Structure-Based Virtual Screening. *Journal of Chemical Information and Modeling*, **2017**, 57, 1474-1487	6.1	35
239	Comparative analyses of structural features and scaffold diversity for purchasable compound libraries. *Journal of Cheminformatics*, **2017**, 9, 25	8.6	17
238	Controlling of the electronic properties of WS2 and graphene oxide heterostructures from first-principles calculations. *Journal of Materials Chemistry C*, **2017**, 5, 201-207	7.1	11
237	ADMET Evaluation in Drug Discovery. Part 17: Development of Quantitative and Qualitative Prediction Models for Chemical-Induced Respiratory Toxicity. *Molecular Pharmaceutics*, **2017**, 14, 2407-2421	5.6	42
236	Improving the Efficiency of Non-equilibrium Sampling in the Aqueous Environment via Implicit-Solvent Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 1827-1836	6.4	5
235	Exploring the RNA-bound and RNA-free human Argonaute-2 by molecular dynamics simulation method. *Chemical Biology and Drug Design*, **2017**, 90, 753-763	2.9	4
234	Prediction of luciferase inhibitors by the high-performance MIEC-GBDT approach based on interaction energetic patterns. *Physical Chemistry Chemical Physics*, **2017**, 19, 10163-10176	3.6	21
233	Two-dimensional germanium monochalcogenide photocatalyst for water splitting under ultraviolet, visible to near-infrared light. *Nanoscale*, **2017**, 9, 8608-8615	7.7	85
232	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
231	A novel metal-free two-dimensional material for photocatalytic water splitting phosphorus nitride (PN). *RSC Advances*, **2017**, 7, 50239-50245	3.7	22
230	ADMET Evaluation in Drug Discovery. 18. Reliable Prediction of Chemical-Induced Urinary Tract Toxicity by Boosting Machine Learning Approaches. *Molecular Pharmaceutics*, **2017**, 14, 3935-3953	5.6	46

229	HawkRank: a new scoring function for protein-protein docking based on weighted energy terms. *Journal of Cheminformatics*, **2017**, 9, 66	8.6	31
228	How Does the L884P Mutation Confer Resistance to Type-II Inhibitors of JAK2 Kinase: A Comprehensive Molecular Modeling Study. *Scientific Reports*, **2017**, 7, 9088	4.9	15
227	Two-dimensional porous polyphthalocyanine (PPc) as an efficient gas-separation membrane for ammonia synthesis. *Current Applied Physics*, **2017**, 17, 1765-1770	2.6	4
226	Discovery of a ROCK inhibitor, FPND, which prevents cerebral hemorrhage through maintaining vascular integrity by interference with VE-cadherin. *Cell Death Discovery*, **2017**, 3, 17051	6.9	12
225	Aggregated Single-Walled Carbon Nanotubes Absorb and Deform Dopamine-Related Proteins Based on Molecular Dynamics Simulations. *ACS Applied Materials & Interfaces*, **2017**, 9, 32452-32462	9.5	16
224	Characterizing Drug-Target Residence Time with Metadynamics: How To Achieve Dissociation Rate Efficiently without Losing Accuracy against Time-Consuming Approaches. *Journal of Chemical Information and Modeling*, **2017**, 57, 1895-1906	6.1	28
223	Combating Drug-Resistant Mutants of Anaplastic Lymphoma Kinase with Potent and Selective Type-I Inhibitors by Stabilizing Unique DFG-Shifted Loop Conformation. *ACS Central Science*, **2017**, 3, 1208-1220	16.8	30
222	Monolayer germanium monochalcogenides (GeS/GeSe) as cathode catalysts in nonaqueous Li-O batteries. *Physical Chemistry Chemical Physics*, **2017**, 19, 20457-20462	3.6	30
221	Theoretical investigations on novel SiC5 siligraphene as gas sensor for air pollutants. *Carbon*, **2017**, 113, 114-121	10.4	48
220	Structural Diversity of Ligand-Binding Androgen Receptors Revealed by Microsecond Long Molecular Dynamics Simulations and Enhanced Sampling. *Journal of Chemical Theory and Computation*, **2016**, 12, 4611-9	6.4	39
219	Inhibition of macrophage migration inhibitory factor (MIF) tautomerase activity suppresses microglia-mediated inflammatory responses. *Clinical and Experimental Pharmacology and Physiology* , **2016**, 43, 1134-1144	3	20
218	In Silico Exploration for Novel Type-I Inhibitors of Tie-2/TEK: The Performance of Different Selection Strategy in Selecting Virtual Screening Candidates. *Scientific Reports*, **2016**, 6, 37628	4.9	3
217	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
216	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
215	Atomistic molecular dynamics simulations of ATP-binding cassette transporters. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 255-265	7.9	4
214	Stable and metallic borophene nanoribbons from first-principles calculations. *Journal of Materials Chemistry C*, **2016**, 4, 6380-6385	7.1	59
213	Discovery of a novel ROCK2 inhibitor with anti-migration effects via docking and high-content drug screening. *Molecular BioSystems*, **2016**, 12, 2713-21		9
212	B40 fullerene as a highly sensitive molecular device for NH3 detection at low bias: a first-principles study. *Nanotechnology*, **2016**, 27, 075501	3.4	34

211	Binding mechanisms of 1,4-dihydropyridine derivatives to L-type calcium channel Cav1.2: a molecular modeling study. *Molecular BioSystems*, **2016**, 12, 379-90		17
210	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
209	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
208	SiC7 siligraphene: a novel donor material with extraordinary sunlight absorption. *Nanoscale*, **2016**, 8, 6994-9	7.7	54
207	Molecular principle of the cyclin-dependent kinase selectivity of 4-(thiazol-5-yl)-2-(phenylamino) pyrimidine-5-carbonitrile derivatives revealed by molecular modeling studies. *Physical Chemistry Chemical Physics*, **2016**, 18, 2034-46	3.6	17
206	A novel small molecule agent displays potent anti-myeloma activity by inhibiting the JAK2-STAT3 signaling pathway. *Oncotarget*, **2016**, 7, 9296-308	3.3	19
205	Recent Advances in Protein-Protein Docking. *Current Drug Targets*, **2016**, 17, 1586-1594	3	15
204	Ab initio phonon-coupled nonadiabatic relaxation dynamics of [Au25(SH)18]□clusters. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 458-462	1.3	11
203	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
202	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
201	Heptazine-based graphitic carbon nitride as an effective hydrogen purification membrane. *RSC Advances*, **2016**, 6, 52377-52383	3.7	52
200	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
199	CaFE: a tool for binding affinity prediction using end-point free energy methods. *Bioinformatics*, **2016**, 32, 2216-8	7.2	48
198	Characterising the morphology and efficiency of polymer solar cell by experiments and simulations. *Molecular Simulation*, **2016**, 42, 836-845	2	8
197	Exploring the molecular basis of RNA recognition by the dimeric RNA-binding protein via molecular simulation methods. *RNA Biology*, **2016**, 13, 1133-1143	4.8	14
196	DNA-PKcs, a novel functional target of acriflavine, mediates acriflavine's p53-dependent synergistic anti-tumor efficiency with melphalan. *Cancer Letters*, **2016**, 383, 115-124	9.9	8
195	Lithium intercalation and diffusion in TiO2 nanotubes: a first-principles investigation. *Physical Chemistry Chemical Physics*, **2016**, 18, 24370-6	3.6	16
194	Exploring resistance mechanisms of HCV NS3/4A protease mutations to MK5172: insight from molecular dynamics simulations and free energy calculations. *Molecular BioSystems*, **2015**, 11, 2568-78		15

193	Semiconducting Graphene on Silicon from First-Principles Calculations. *ACS Nano*, **2015**, 9, 8562-8	16.7	20
192	B40 fullerene: An efficient material for CO2 capture, storage and separation. *Current Applied Physics*, **2015**, 15, 1084-1089	2.6	60
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