Ting-Jun Hou

List of Publications by Year
in descending order

373	23,519	9234	12233
papers	citations	74 h-index	133 g-index

383	383	383	20225
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Kinome-wide polypharmacology profiling of small molecules by multi-task graph isomorphism network approach. Acta Pharmaceutica Sinica B, 2023, 13, 54-67.	5.7	9
2	Discovery of novel antagonists targeting the DNA binding domain of androgen receptor by integrated docking-based virtual screening and bioassays. Acta Pharmacologica Sinica, 2022, 43, 229-239.	2.8	14
3	Discovery of novel MIF inhibitors that attenuate microglial inflammatory activation by structures-based virtual screening and in vitro bioassays. Acta Pharmacologica Sinica, 2022, 43, 1508-1520.	2.8	10
4	Featurization strategies for proteinâ€“ligand interactions and their applications in scoring function development. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1567.	6.2	24
5	Molecular View on the Dissociation Pathways and Transactivation Regulation Mechanism of Nonsteroidal GR Ligands. Journal of Chemical Information and Modeling, 2022, 62, 5233-5245.	2.5	5
6	DDInter: an online drugâ€“drug interaction database towards improving clinical decision-making and patient safety. Nucleic Acids Research, 2022, 50, D1200-D1207.	6.5	37
7	Discovery of novel DprE1 inhibitors via computational bioactivity fingerprints and structure-based virtual screening. Acta Pharmacologica Sinica, 2022, 43, 1605-1615.	2.8	6
8	Deep learning approaches for de novo drug design: An overview. Current Opinion in Structural Biology, 2022, 72, 135-144.	2.6	54
9	Discovery of Novel GR Ligands toward Druggable GR Antagonist Conformations Identified by MD Simulations and Markov State Model Analysis. Advanced Science, 2022, 9, e2102435.	5.6	28
10	Out-of-the-box deep learning prediction of quantum-mechanical partial charges by graph representation and transfer learning. Briefings in Bioinformatics, 2022, 23, .	3.2	7
11	Discovery of N-(4-(Benzyloxy)-phenyl)-sulfonamide Derivatives as Novel Antagonists of the Human Androgen Receptor Targeting the Activation Function 2. Journal of Medicinal Chemistry, 2022, 65, 2507-2521.	2.9	8
12	ABC-Net: a divide-and-conquer based deep learning architecture for SMILES recognition from molecular images. Briefings in Bioinformatics, 2022, 23, .	3.2	7
13	Discovery of a novel nonsteroidal selective glucocorticoid receptor modulator by virtual screening and bioassays. Acta Pharmacologica Sinica, 2022, 43, 2429-2438.	2.8	11
14	Knowledge-based BERT: a method to extract molecular features like computational chemists. Briefings in Bioinformatics, 2022, 23, .	3.2	24
15	High-throughput glycolytic inhibitor discovery targeting glioblastoma by graphite dotsâ€“assisted LDI mass spectrometry. Science Advances, 2022, 8, eabl4923.	4.7	14
16	The structure of erastin-bound xCTâ€“4F2hc complexÂreveals molecular mechanisms underlying erastin-induced ferroptosis. Cell Research, 2022, 32, 687-690.	5.7	48
17	Characterizing the stabilization effects of stabilizers in proteinâ€“protein systems with end-point binding free energy calculations. Briefings in Bioinformatics, 2022, 23, .	3.2	10
18	Comprehensive assessment of deep generative architectures for de novo drug design. Briefings in Bioinformatics, 2022, 23, .	3.2	9

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19	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.	2.6	8
20	Machine learning to predict metabolic drug interactions related to cytochrome P450 isozymes. Journal of Cheminformatics, 2022, 14, 23.	2.8	14
21	fastDRH: a webserver to predict and analyze proteinâ€“ligand complexes based on molecular docking and MM/PB(GB)SA computation. Briefings in Bioinformatics, 2022, 23, .	3.2	34
22	Novel Caspase-1 inhibitor CZL80 improves neurological function in mice after progressive ischemic stroke within a long therapeutic time-window. Acta Pharmacologica Sinica, 2022, 43, 2817-2827.	2.8	6
23	TocoDecoy: A New Approach to Design Unbiased Datasets for Training and Benchmarking Machine-Learning Scoring Functions. Journal of Medicinal Chemistry, 2022, 65, 7918-7932.	2.9	12
24	Organic Compound Synthetic Accessibility Prediction Based on the Graph Attention Mechanism. Journal of Chemical Information and Modeling, 2022, 62, 2973-2986.	2.5	11
25	RELATION: A Deep Generative Model for Structure-Based De Novo Drug Design. Journal of Medicinal Chemistry, 2022, 65, 9478-9492.	2.9	36
26	Root-aligned SMILES: a tight representation for chemical reaction prediction. Chemical Science, 2022, 13, 9023-9034.	3.7	17
27	ChemFLuo: a web-server for structure analysis and identification of fluorescent compounds. Briefings in Bioinformatics, 2021, 22, .	3.2	4
28	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, .	3.2	70
29	Beware of the generic machine learning-based scoring functions in structure-based virtual screening. Briefings in Bioinformatics, 2021, 22, .	3.2	39
30	Improving structure-based virtual screening performance via learning from scoring function components. Briefings in Bioinformatics, 2021, 22, .	3.2	28
31	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.	3.2	49
32	PROTAC-DB: an online database of PROTACs. Nucleic Acids Research, 2021, 49, D1381-D1387.	6.5	127
33	CovalentInDB: a comprehensive database facilitating the discovery of covalent inhibitors. Nucleic Acids Research, 2021, 49, D1122-D1129.	6.5	42
34	Current advances in ligandâ€based target prediction. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1504.	6.2	20
35	Targeting phosphatidylinositol 3â€kinase gamma (PI3Kî³): Discovery and development of its selective inhibitors. Medicinal Research Reviews, 2021, 41, 1599-1621.	5.0	21
36	Scopy: an integrated negative design python library for desirable HTS/VS database design. Briefings in Bioinformatics, 2021, 22, .	3.2	21

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37	DeepAtomicCharge: a new graph convolutional network-based architecture for accurate prediction of atomic charges. Briefings in Bioinformatics, 2021, 22, .	3.2	16
38	BioMedR: an R/CRAN package for integrated data analysis pipeline in biomedical study. Briefings in Bioinformatics, 2021, 22, 474-484.	3.2	8
39	Accuracy or novelty: what can we gain from target-specific machine-learning-based scoring functions in virtual screening?. Briefings in Bioinformatics, 2021, 22, .	3.2	26
40	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.	2.8	214
41	ASFP (Artificial Intelligence based Scoring Function Platform): a web server for the development of customized scoring functions. Journal of Cheminformatics, 2021, 13, 6.	2.8	8
42	PySmash: Python package and individual executable program for representative substructure generation and application. Briefings in Bioinformatics, 2021, 22, .	3.2	6
43	Hyperbolic relational graph convolution networks plus: a simple but highly efficient QSAR-modeling method. Briefings in Bioinformatics, 2021, 22, .	3.2	22
44	ADMETlab 2.0: an integrated online platform for accurate and comprehensive predictions of ADMET properties. Nucleic Acids Research, 2021, 49, W5-W14.	6.5	915
45	Cover Image, Volume 11, Issue 3. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1533.	6.2	0
46	ARIH1 signaling promotes anti-tumor immunity by targeting PD-L1 for proteasomal degradation. Nature Communications, 2021, 12, 2346.	5.8	52
47	Identification of active molecules againstMycobacterium tuberculosisthrough machine learning. Briefings in Bioinformatics, 2021, 22, .	3.2	25
48	Discovery of novel HBV capsid assembly modulators by structure-based virtual screening and bioassays. Bioorganic and Medicinal Chemistry, 2021, 36, 116096.	1.4	9
49	Structural basis of GABAB receptorâ€“Gi protein coupling. Nature, 2021, 594, 594-598.	13.7	50
50	VAD-MM/GBSA: A Variable Atomic Dielectric MM/GBSA Model for Improved Accuracy in Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2844-2856.	2.5	29
51	Computational Bioactivity Fingerprint Similarities To Navigate the Discovery of Novel Scaffolds. Journal of Medicinal Chemistry, 2021, 64, 7544-7554.	2.9	12
52	Mining Toxicity Information from Large Amounts of Toxicity Data. Journal of Medicinal Chemistry, 2021, 64, 6924-6936.	2.9	39
53	The MCR-3 inside linker appears as a facilitator of colistin resistance. Cell Reports, 2021, 35, 109135.	2.9	15
54	DeepChargePredictor: a web server for predicting QM-based atomic charges via state-of-the-art machine-learning algorithms. Bioinformatics, 2021, 37, 4255-4257.	1.8	4

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55	MG-BERT: leveraging unsupervised atomic representation learning for molecular property prediction. Briefings in Bioinformatics, 2021, 22, .	3.2	62
56	Benchmarking the mechanisms of frequent hitters: limitation of PAINS alerts. Drug Discovery Today, 2021, 26, 1353-1358.	3.2	15
57	Metformin activates chaperone-mediated autophagy and improves disease pathologies in an Alzheimer disease mouse model. Protein and Cell, 2021, 12, 769-787.	4.8	63
58	Discovery of a small molecule inhibitor of cullin neddylation that triggers ER stress to induce autophagy. Acta Pharmaceutica Sinica B, 2021, 11, 3567-3584.	5.7	16
59	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.	2.1	12
60	Structural insights into ligand recognition and activation of the melanocortin-4 receptor. Cell Research, 2021, 31, 1163-1175.	5.7	26
61	Learning to SMILES: BAN-based strategies to improve latent representation learning from molecules. Briefings in Bioinformatics, 2021, 22, .	3.2	25
62	Discovery of a Novel Fusarium Graminearum Mitogen-Activated Protein Kinase (FgGpmk1) Inhibitor for the Treatment of Fusarium Head Blight. Journal of Medicinal Chemistry, 2021, 64, 13841-13852.	2.9	7
63	Opportunities for overcoming tuberculosis: Emerging targets and their inhibitors. Drug Discovery Today, 2021, 27, 326-326.	3.2	13
64	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.	1.7	5
65	Characterizing the Morphology and Efficiency of Organic Solar Cells by Multiscale Simulations. Springer Series in Materials Science, 2021, , 679-692.	0.4	0
66	QSAR-assisted-MMPA to expand chemical transformation space for lead optimization. Briefings in Bioinformatics, 2021, 22, .	3.2	10
67	The impact of cross-docked poses on performance of machine learning classifier for proteinâ€“ligand binding pose prediction. Journal of Cheminformatics, 2021, 13, 81.	2.8	18
68	Multi-constraint molecular generation based on conditional transformer, knowledge distillation and reinforcement learning. Nature Machine Intelligence, 2021, 3, 914-922.	8.3	73
69	Integrative Modeling of PROTAC-Mediated Ternary Complexes. Journal of Medicinal Chemistry, 2021, 64, 16271-16281.	2.9	51
70	Pterostilbene inhibits hepatocellular carcinoma proliferation and HBV replication by targeting ribonucleotide reductase M2 protein. American Journal of Cancer Research, 2021, 11, 2975-2989.	1.4	1
71	A unified drugâ€“target interaction prediction framework based on knowledge graph and recommendation system. Nature Communications, 2021, 12, 6775.	5.8	86
72	Semi-automated workflow for molecular pair analysis and QSAR-assisted transformation space expansion. Journal of Cheminformatics, 2021, 13, 86.	2.8	3

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73	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.	2.9	7
74	InteractionGraphNet: A Novel and Efficient Deep Graph Representation Learning Framework for Accurate Proteinâ€“Ligand Interaction Predictions. Journal of Medicinal Chemistry, 2021, 64, 18209-18232.	2.9	87
75	From machine learning to deep learning: Advances in scoring functions for proteinâ€“ligand docking. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1429.	6.2	142
76	Combined strategies in structure-based virtual screening. Physical Chemistry Chemical Physics, 2020, 22, 3149-3159.	1.3	83
77	Application of Negative Design To Design a More Desirable Virtual Screening Library. Journal of Medicinal Chemistry, 2020, 63, 4411-4429.	2.9	19
78	Systematic Modeling of logâ€¯D_{7.4} Based on Ensemble Machine Learning, Group Contribution, and Matched Molecular Pair Analysis. Journal of Chemical Information and Modeling, 2020, 60, 63-76.	2.5	36
79	Insight Derived from Molecular Dynamics Simulation into the Selectivity Mechanism Targeting c-MYC G-Quadruplex. Journal of Physical Chemistry B, 2020, 124, 9773-9784.	1.2	7
80	Fast and accurate prediction of partial charges using Atom-Path-Descriptor-based machine learning. Bioinformatics, 2020, 36, 4721-4728.	1.8	9
81	Development and Evaluation of MM/GBSA Based on a Variable Dielectric GB Model for Predicting Proteinâ€“Ligand Binding Affinities. Journal of Chemical Information and Modeling, 2020, 60, 5353-5365.	2.5	25
82	Gossypol inhibits cullin neddylation by targeting SAG-CUL5 and RBX1-CUL1 complexes. Neoplasia, 2020, 22, 179-191.	2.3	17
83	Structural Analysis and Identification of False Positive Hits in Luciferase-Based Assays. Journal of Chemical Information and Modeling, 2020, 60, 2031-2043.	2.5	17
84	ADMET evaluation in drug discovery. 20. Prediction of breast cancer resistance protein inhibition through machine learning. Journal of Cheminformatics, 2020, 12, 16.	2.8	45
85	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.	1.3	9
86	Novel androgen receptor antagonist identified by structure-based virtual screening, structural optimization, and biological evaluation. European Journal of Medicinal Chemistry, 2020, 192, 112156.	2.6	15
87	Frequent hitters: nuisance artifacts in high-throughput screening. Drug Discovery Today, 2020, 25, 657-667.	3.2	33
88	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.	2.5	40
89	Structureâ€based discovery of CZL80, a caspaseâ€1 inhibitor with therapeutic potential for febrile seizures and later enhanced epileptogenic susceptibility. British Journal of Pharmacology, 2020, 177, 3519-3534.	2.7	26
90	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.	1.0	12

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91	Comprehensive Evaluation of Fourteen Docking Programs on Proteinâ€“Peptide Complexes. Journal of Chemical Theory and Computation, 2020, 16, 3959-3969.	2.3	90
92	Advances in the computational development of androgen receptor antagonists. Drug Discovery Today, 2020, 25, 1453-1461.	3.2	21
93	Cover Image, Volume 39, Issue 5. Medicinal Research Reviews, 2019, 39, i-i.	5.0	0
94	Assessing the performance of the MM/PBSA and MM/GBSA methods. 10. Impacts of enhanced sampling and variable dielectric model on proteinâ€“protein Interactions. Physical Chemistry Chemical Physics, 2019, 21, 18958-18969.	1.3	80
95	Drug Discovery Targeting Anaplastic Lymphoma Kinase (ALK). Journal of Medicinal Chemistry, 2019, 62, 10927-10954.	2.9	80
96	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.	2.5	85
97	DNA methyltransferases: emerging targets for the discovery of inhibitors as potent anticancer drugs. Drug Discovery Today, 2019, 24, 2323-2331.	3.2	46
98	Structural Analysis and Identification of Colloidal Aggregators in Drug Discovery. Journal of Chemical Information and Modeling, 2019, 59, 3714-3726.	2.5	41
99	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.	1.0	14
100	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.	2.5	30
101	Voltage-gated sodium channels: structures, functions, and molecular modeling. Drug Discovery Today, 2019, 24, 1389-1397.	3.2	36
102	End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. Chemical Reviews, 2019, 119, 9478-9508.	23.0	1,064
103	Insight into the selective binding mechanism of DNMT1 and DNMT3A inhibitors: a molecular simulation study. Physical Chemistry Chemical Physics, 2019, 21, 12931-12947.	1.3	39
104	HawkDock: a web server to predict and analyze the proteinâ€“protein complex based on computational docking and MM/GBSA. Nucleic Acids Research, 2019, 47, W322-W330.	6.5	329
105	Assessing the performance of MM/PBSA and MM/GBSA methods. 9. Prediction reliability of binding affinities and binding poses for proteinâ€“peptide complexes. Physical Chemistry Chemical Physics, 2019, 21, 10135-10145.	1.3	96
106	Increased gene copy number of DEFA1/DEFA3 worsens sepsis by inducing endothelial pyroptosis. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3161-3170.	3.3	41
107	The inflammatory cytokine IL-6 induces FRA1 deacetylation promoting colorectal cancer stem-like properties. Oncogene, 2019, 38, 4932-4947.	2.6	48
108	Importance of a crystalline water network in docking-based virtual screening: a case study of BRD4. Physical Chemistry Chemical Physics, 2019, 21, 25276-25289.	1.3	19

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109	Identification of an Activating Mutation in the Extracellular Domain of HER2 Conferring Resistance to Pertuzumab . OncoTargets and Therapy, 2019, Volume 12, 11597-11608.	1.0	12
110	A magic drug target: Androgen receptor. Medicinal Research Reviews, 2019, 39, 1485-1514.	5.0	44
111	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.	1.8	59
112	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.	3.1	26
113	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.	1.7	23
114	Fullerene derivatives act as inhibitors of leukocyte common antigen based on molecular dynamics simulations. RSC Advances, 2018, 8, 13997-14008.	1.7	10
115	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.	1.1	13
116	Benchmark Study Based on 2P2I_{DB} to Gain Insights into the Discovery of Small-Molecule PPI Inhibitors. Journal of Physical Chemistry B, 2018, 122, 2544-2555.	1.2	12
117	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.	1.3	22
118	Janus Structures of Transition Metal Dichalcogenides as the Heterojunction Photocatalysts for Water Splitting. Journal of Physical Chemistry C, 2018, 122, 3123-3129.	1.5	246
119	Monolayer graphitic germanium carbide (g-GeC): the promising cathode catalyst for fuel cell and lithiumâ€“oxygen battery applications. Journal of Materials Chemistry A, 2018, 6, 2212-2218.	5.2	70
120	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.	1.3	243
121	Two-dimensional siligraphenes as cathode catalysts for nonaqueous lithium-oxygen batteries. Carbon, 2018, 126, 580-587.	5.4	40
122	Discovery of Novel Androgen Receptor Ligands by Structure-based Virtual Screening and Bioassays. Genomics, Proteomics and Bioinformatics, 2018, 16, 416-427.	3.0	32
123	Origin of the catalytic activity of phosphorus doped MoS2 for oxygen reduction reaction (ORR) in alkaline solution: a theoretical study. Scientific Reports, 2018, 8, 13292.	1.6	20
124	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, , .	3.2	16
125	Structure-Based Drug Design and Identification of H₂O-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.	2.9	27
126	Cheminformatic Insight into the Differences between Terrestrial and Marine Originated Natural Products. Journal of Chemical Information and Modeling, 2018, 58, 1182-1193.	2.5	45

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127	Assessing the performance of MM/PBSA and MM/GBSA methods. 8. Predicting binding free energies and poses of proteinâ€“RNA complexes. Rna, 2018, 24, 1183-1194.	1.6	84
128	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.	2.5	37
129	Peptide-Tethered Hydrogel Scaffold Promotes Recovery from Spinal Cord Transection via Synergism with Mesenchymal Stem Cells. ACS Applied Materials & Interfaces, 2017, 9, 3330-3342.	4.0	90
130	Atomistic Origins of Surface Defects in CH₃NH₃PbBr₃ Perovskite and Their Electronic Structures. ACS Nano, 2017, 11, 2060-2065.	7.3	123
131	Discovery of Novel and Selective Adenosine A_{2A} Receptor Antagonists for Treating Parkinsonâ€™s Disease through Comparative Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1474-1487.	2.5	45
132	Comparative analyses of structural features and scaffold diversity for purchasable compound libraries. Journal of Cheminformatics, 2017, 9, 25.	2.8	25
133	Controlling of the electronic properties of WS₂ and graphene oxide heterostructures from first-principles calculations. Journal of Materials Chemistry C, 2017, 5, 201-207.	2.7	16
134	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.	2.3	59
135	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.	2.3	6
136	Exploring the RNAâ€bound and RNAâ€free human Argonauteâ€2 by molecular dynamics simulation method. Chemical Biology and Drug Design, 2017, 90, 753-763.	1.5	9
137	Prediction of luciferase inhibitors by the high-performance MIEC-GBDT approach based on interaction energetic patterns. Physical Chemistry Chemical Physics, 2017, 19, 10163-10176.	1.3	27
138	Two-dimensional germanium monochalcogenide photocatalyst for water splitting under ultraviolet, visible to near-infrared light. Nanoscale, 2017, 9, 8608-8615.	2.8	124
139	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.	5.2	53
140	A novel metal-free two-dimensional material for photocatalytic water splitting â€“ phosphorus nitride (Î³-PN). RSC Advances, 2017, 7, 50239-50245.	1.7	26
141	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.	2.3	66
142	Two-dimensional porous polyphthalocyanine (PPc) as an efficient gas-separation membrane for ammonia synthesis. Current Applied Physics, 2017, 17, 1765-1770.	1.1	5
143	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.	2.0	16
144	Aggregated Single-Walled Carbon Nanotubes Absorb and Deform Dopamine-Related Proteins Based on Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 32452-32462.	4.0	24

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145	Characterizing Drugâ€“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.	2.5	53
146	Combating Drug-Resistant Mutants of Anaplastic Lymphoma Kinase with Potent and Selective Type-I^{1/2} Inhibitors by Stabilizing Unique DFG-Shifted Loop Conformation. ACS Central Science, 2017, 3, 1208-1220.	5.3	42
147	Monolayer germanium monochalcogenides (GeS/GeSe) as cathode catalysts in nonaqueous Liâ€“O₂batteries. Physical Chemistry Chemical Physics, 2017, 19, 20457-20462.	1.3	36
148	Theoretical investigations on novel SiC5 siligraphene as gas sensor for air pollutants. Carbon, 2017, 113, 114-121.	5.4	64
149	HawkRank: a new scoring function for proteinâ€“protein docking based on weighted energy terms. Journal of Cheminformatics, 2017, 9, 66.	2.8	48
150	How Does the L884P Mutation Confer Resistance to Type-II Inhibitors of JAK2 Kinase: A Comprehensive Molecular Modeling Study. Scientific Reports, 2017, 7, 9088.	1.6	16
151	Ab initio phononâ€coupled nonadiabatic relaxation dynamics of [Au 25 (SH) 18] â^' clusters. Physica Status Solidi (B): Basic Research, 2016, 253, 458-462.	0.7	12
152	ADMET Evaluation in Drug Discovery. 16. Predicting hERG Blockers by Combining Multiple Pharmacophores and Machine Learning Approaches. Molecular Pharmaceutics, 2016, 13, 2855-2866.	2.3	90
153	Constructing and Validating High-Performance MIEC-SVM Models in Virtual Screening for Kinases: A Better Way for Actives Discovery. Scientific Reports, 2016, 6, 24817.	1.6	59
154	Heptazine-based graphitic carbon nitride as an effective hydrogen purification membrane. RSC Advances, 2016, 6, 52377-52383.	1.7	76
155	Comprehensive evaluation of ten docking programs on a diverse set of proteinâ€“ligand complexes: the prediction accuracy of sampling power and scoring power. Physical Chemistry Chemical Physics, 2016, 18, 12964-12975.	1.3	669
156	CaFE: a tool for binding affinity prediction using end-point free energy methods. Bioinformatics, 2016, 32, 2216-2218.	1.8	114
157	Characterising the morphology and efficiency of polymer solar cell by experiments and simulations. Molecular Simulation, 2016, 42, 836-845.	0.9	9
158	Exploring the molecular basis of RNA recognition by the dimeric RNA-binding protein via molecular simulation methods. RNA Biology, 2016, 13, 1133-1143.	1.5	18
159	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.	3.2	11
160	Lithium intercalation and diffusion in TiO₂ nanotubes: a first-principles investigation. Physical Chemistry Chemical Physics, 2016, 18, 24370-24376.	1.3	24
161	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, 4611-4619.	2.3	51
162	Inhibition of macrophage migration inhibitory factor (<scp>MIF</scp>) tautomerase activity suppresses microgliaâ€mediated inflammatory responses. Clinical and Experimental Pharmacology and Physiology, 2016, 43, 1134-1144.	0.9	39

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