List of Publications by Year in descending order

263 papers	20,213 citations	12322 69 h-index	13758 129 g-index
268 all docs	268 docs citations	268 times ranked	16724 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	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
3	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
4	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
5	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
6	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
7	Knowledge-based BERT: a method to extract molecular features like computational chemists. Briefings in Bioinformatics, 2022, 23, .	3.2	24
8	High-throughput glycolytic inhibitor discovery targeting glioblastoma by graphite dotsâ€“assisted LDI mass spectrometry. Science Advances, 2022, 8, eabl4923.	4.7	14
9	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
10	Comprehensive assessment of deep generative architectures for de novo drug design. Briefings in Bioinformatics, 2022, 23, .	3.2	9
11	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
12	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
13	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
14	Organic Compound Synthetic Accessibility Prediction Based on the Graph Attention Mechanism. Journal of Chemical Information and Modeling, 2022, 62, 2973-2986.	2.5	11
15	RELATION: A Deep Generative Model for Structure-Based De Novo Drug Design. Journal of Medicinal Chemistry, 2022, 65, 9478-9492.	2.9	36
16	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
17	Beware of the generic machine learning-based scoring functions in structure-based virtual screening. Briefings in Bioinformatics, 2021, 22, .	3.2	39
18	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

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19	PROTAC-DB: an online database of PROTACs. Nucleic Acids Research, 2021, 49, D1381-D1387.	6.5	127
20	Targeting phosphatidylinositol 3â€kinase gamma (PI3KÎ³): Discovery and development of its selective inhibitors. Medicinal Research Reviews, 2021, 41, 1599-1621.	5.0	21
21	DeepAtomicCharge: a new graph convolutional network-based architecture for accurate prediction of atomic charges. Briefings in Bioinformatics, 2021, 22, .	3.2	16
22	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
23	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
24	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
25	Hyperbolic relational graph convolution networks plus: a simple but highly efficient QSAR-modeling method. Briefings in Bioinformatics, 2021, 22, .	3.2	22
26	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
27	Identification of active molecules againstMycobacterium tuberculosisthrough machine learning. Briefings in Bioinformatics, 2021, 22, .	3.2	25
28	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
29	Mining Toxicity Information from Large Amounts of Toxicity Data. Journal of Medicinal Chemistry, 2021, 64, 6924-6936.	2.9	39
30	The MCR-3 inside linker appears as a facilitator of colistin resistance. Cell Reports, 2021, 35, 109135.	2.9	15
31	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
32	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
33	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
34	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
35	Characterizing the Morphology and Efficiency of Organic Solar Cells by Multiscale Simulations. Springer Series in Materials Science, 2021, , 679-692.	0.4	0
36	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

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37	Multi-constraint molecular generation based on conditional transformer, knowledge distillation and reinforcement learning. Nature Machine Intelligence, 2021, 3, 914-922.	8.3	73
38	Integrative Modeling of PROTAC-Mediated Ternary Complexes. Journal of Medicinal Chemistry, 2021, 64, 16271-16281.	2.9	51
39	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
40	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
41	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
42	Combined strategies in structure-based virtual screening. Physical Chemistry Chemical Physics, 2020, 22, 3149-3159.	1.3	83
43	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
44	Fast and accurate prediction of partial charges using Atom-Path-Descriptor-based machine learning. Bioinformatics, 2020, 36, 4721-4728.	1.8	9
45	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
46	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
47	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
48	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
49	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
50	Comprehensive Evaluation of Fourteen Docking Programs on Proteinâ€“Peptide Complexes. Journal of Chemical Theory and Computation, 2020, 16, 3959-3969.	2.3	90
51	Advances in the computational development of androgen receptor antagonists. Drug Discovery Today, 2020, 25, 1453-1461.	3.2	21
52	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
53	Drug Discovery Targeting Anaplastic Lymphoma Kinase (ALK). Journal of Medicinal Chemistry, 2019, 62, 10927-10954.	2.9	80
54	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

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55	DNA methyltransferases: emerging targets for the discovery of inhibitors as potent anticancer drugs. Drug Discovery Today, 2019, 24, 2323-2331.	3.2	46
56	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
57	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
58	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
59	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
60	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
61	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
62	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
63	The inflammatory cytokine IL-6 induces FRA1 deacetylation promoting colorectal cancer stem-like properties. Oncogene, 2019, 38, 4932-4947.	2.6	48
64	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
65	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
66	A magic drug target: Androgen receptor. Medicinal Research Reviews, 2019, 39, 1485-1514.	5.0	44
67	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
68	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
69	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
70	Fullerene derivatives act as inhibitors of leukocyte common antigen based on molecular dynamics simulations. RSC Advances, 2018, 8, 13997-14008.	1.7	10
71	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
72	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

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73	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
74	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
75	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
76	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
77	Two-dimensional siligraphenes as cathode catalysts for nonaqueous lithium-oxygen batteries. Carbon, 2018, 126, 580-587.	5.4	40
78	Discovery of Novel Androgen Receptor Ligands by Structure-based Virtual Screening and Bioassays. Genomics, Proteomics and Bioinformatics, 2018, 16, 416-427.	3.0	32
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	Comparative analyses of structural features and scaffold diversity for purchasable compound libraries. Journal of Cheminformatics, 2017, 9, 25.	2.8	25
87	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
88	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
89	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
90	Two-dimensional germanium monochalcogenide photocatalyst for water splitting under ultraviolet, visible to near-infrared light. Nanoscale, 2017, 9, 8608-8615.	2.8	124

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91	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
92	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
93	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
94	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
95	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
96	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
97	Monolayer germanium monochalcogenides (GeS/GeSe) as cathode catalysts in nonaqueous Liâ€“O₂batteries. Physical Chemistry Chemical Physics, 2017, 19, 20457-20462.	1.3	36
98	Theoretical investigations on novel SiC5 siligraphene as gas sensor for air pollutants. Carbon, 2017, 113, 114-121.	5.4	64
99	HawkRank: a new scoring function for proteinâ€“protein docking based on weighted energy terms. Journal of Cheminformatics, 2017, 9, 66.	2.8	48
100	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
101	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
102	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
103	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
104	CaFE: a tool for binding affinity prediction using end-point free energy methods. Bioinformatics, 2016, 32, 2216-2218.	1.8	114
105	Characterising the morphology and efficiency of polymer solar cell by experiments and simulations. Molecular Simulation, 2016, 42, 836-845.	0.9	9
106	Lithium intercalation and diffusion in TiO₂ nanotubes: a first-principles investigation. Physical Chemistry Chemical Physics, 2016, 18, 24370-24376.	1.3	24
107	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
108	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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109	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.	1.6	4
110	Potential Application of Novel Boron-Doped Graphene Nanoribbon as Oxygen Reduction Reaction Catalyst. Journal of Physical Chemistry C, 2016, 120, 17427-17434.	1.5	131
111	Assessing the performance of the MM/PBSA and MM/GBSA methods. 6. Capability to predict proteinâ€“protein binding free energies and re-rank binding poses generated by proteinâ€“protein docking. Physical Chemistry Chemical Physics, 2016, 18, 22129-22139.	1.3	350
112	Atomistic molecular dynamics simulations of <scp>ATP</scp>â€binding cassette transporters. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 255-265.	6.2	4
113	Discovery of a novel ROCK2 inhibitor with anti-migration effects via docking and high-content drug screening. Molecular BioSystems, 2016, 12, 2713-2721.	2.9	15
114	B₄₀fullerene as a highly sensitive molecular device for NH₃detection at low bias: a first-principles study. Nanotechnology, 2016, 27, 075501.	1.3	39
115	Binding mechanisms of 1,4-dihydropyridine derivatives to L-type calcium channel Ca_v1.2: a molecular modeling study. Molecular BioSystems, 2016, 12, 379-390.	2.9	20
116	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, 851-860.	2.3	41
117	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.	2.8	102
118	SiC₇siligraphene: a novel donor material with extraordinary sunlight absorption. Nanoscale, 2016, 8, 6994-6999.	2.8	70
119	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, 2034-2046.	1.3	21
120	A novel small molecule agent displays potent anti-myeloma activity by inhibiting the JAK2-STAT3 signaling pathway. Oncotarget, 2016, 7, 9296-9308.	0.8	26
121	Recent Advances in Protein-Protein Docking. Current Drug Targets, 2016, 17, 1586-1594.	1.0	25
122	Discovery of Novel ROCK1 Inhibitors via Integrated Virtual Screening Strategy and Bioassays. Scientific Reports, 2015, 5, 16749.	1.6	27
123	Using Hierarchical Virtual Screening To Combat Drug Resistance of the HIV-1 Protease. Journal of Chemical Information and Modeling, 2015, 55, 1400-1412.	2.5	17
124	Identification and Preliminary SAR Analysis of Novel Type-I Inhibitors of TIE-2 via Structure-Based Virtual Screening and Biological Evaluation in in vitro Models. Journal of Chemical Information and Modeling, 2015, 55, 2693-2704.	2.5	9
125	Two-Dimensional MnO₂ as a Better Cathode Material for Lithium Ion Batteries. Journal of Physical Chemistry C, 2015, 119, 28783-28788.	1.5	98
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127	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, 6098-6113.	1.3	48
128	Advances in computationally modeling human oral bioavailability. Advanced Drug Delivery Reviews, 2015, 86, 11-16.	6.6	36
129	Exploring resistance mechanisms of HCV NS3/4A protease mutations to MK5172: insight from molecular dynamics simulations and free energy calculations. Molecular BioSystems, 2015, 11, 2568-2578.	2.9	17
130	Semiconducting Graphene on Silicon from First-Principles Calculations. ACS Nano, 2015, 9, 8562-8568.	7.3	22
131	B40 fullerene: An efficient material for CO2 capture, storage and separation. Current Applied Physics, 2015, 15, 1084-1089.	1.1	71
132	Revealing the favorable dissociation pathway of type II kinase inhibitors via enhanced sampling simulations and two-end-state calculations. Scientific Reports, 2015, 5, 8457.	1.6	72
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134	Editorial. Advanced Drug Delivery Reviews, 2015, 86, 1.	6.6	5
135	Adsorption of metal adatom on nanographene: Computational investigations. Carbon, 2015, 89, 249-259.	5.4	24
136	Prediction of Human Clearance Based on Animal Data and Molecular Properties. Chemical Biology and Drug Design, 2015, 86, 990-997.	1.5	13
137	Discovery of selective phosphatidylinositol 3-kinase inhibitors to treat hematological malignancies. Drug Discovery Today, 2015, 20, 988-994.	3.2	43
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139	The prediction of the morphology and PCE of small molecular organic solar cells. RSC Advances, 2015, 5, 70939-70948.	1.7	9
140	Structureâ€“Activity Relationships and Anti-inflammatory Activities of N-Carbamothioylformamide Analogues as MIF Tautomerase Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 1994-2004.	2.5	6
141	Theoretical investigations on SiC2 siligraphene as promising metal-free catalyst for oxygen reduction reaction. Journal of Power Sources, 2015, 299, 371-379.	4.0	57
142	Absorption, Distribution, Metabolism, Excretion, and Toxicity Evaluation in Drug Discovery. 14. Prediction of Human Pregnane X Receptor Activators by Using Naive Bayesian Classification Technique. Chemical Research in Toxicology, 2015, 28, 116-125.	1.7	29
143	Exploring the binding mechanisms of MIF to CXCR2 using theoretical approaches. Physical Chemistry Chemical Physics, 2015, 17, 3370-3382.	1.3	23
144	A novel PI3K inhibitor PIK-C98 displays potent preclinical activity against multiple myeloma. Oncotarget, 2015, 6, 185-195.	0.8	17

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145	The Selective Interaction between Silica Nanoparticles and Enzymes from Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e107696.	1.1	31
146	P-loop Conformation Governed Crizotinib Resistance in G2032R-Mutated ROS1 Tyrosine Kinase: Clues from Free Energy Landscape. PLoS Computational Biology, 2014, 10, e1003729.	1.5	86
147	The competitive binding between inhibitors and substrates of HCV NS3/4A protease: A general mechanism of drug resistance. Antiviral Research, 2014, 103, 60-70.	1.9	29
148	ADMET Evaluation in Drug Discovery. 13. Development of in Silico Prediction Models for P-Glycoprotein Substrates. Molecular Pharmaceutics, 2014, 11, 716-726.	2.3	96
149	Synthesis and antiproliferative evaluation of 2-hydroxylated (E)-stilbenes. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 5470-5472.	1.0	21
150	Exploring the prominent performance of CX-4945 derivatives as protein kinase CK2 inhibitors by a combined computational study. Molecular BioSystems, 2014, 10, 1196-1210.	2.9	13
151	Discovery of a benzofuran derivative (MBPTA) as a novel ROCK inhibitor that protects against MPP+-induced oxidative stress and cell death in SH-SY5Y cells. Free Radical Biology and Medicine, 2014, 74, 283-293.	1.3	30
152	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, 16719-16729.	1.3	586
153	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, 22035-22045.	1.3	432
154	Discovery of Novel Inhibitors Targeting the Macrophage Migration Inhibitory Factor via Structure-Based Virtual Screening and Bioassays. Journal of Medicinal Chemistry, 2014, 57, 3737-3745.	2.9	66
155	Fast Energy Relaxation by Trap States Decreases Electron Mobility in TiO2 Nanotubes: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2014, 5, 1642-1647.	2.1	31
156	Assessing an Ensemble Docking-Based Virtual Screening Strategy for Kinase Targets by Considering Protein Flexibility. Journal of Chemical Information and Modeling, 2014, 54, 2664-2679.	2.5	96
157	Mechanism of Graphene Oxide as an Enzyme Inhibitor from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2014, 6, 7153-7163.	4.0	95
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