Wei-Wei Xue

List of Publications by Year
in descending order

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91 papers	4,374 citations	109321 35 h-index	118850 62 g-index
95 all docs	95 docs citations	95 times ranked	3950 citing authors

#	Article	IF	Citations
1	NOREVA: normalization and evaluation of MS-based metabolomics data. Nucleic Acids Research, 2017, 45, W162-W170.	14.5	305
2	What Contributes to Serotoninâ€“Norepinephrine Reuptake Inhibitorsâ€™ Dual-Targeting Mechanism? The Key Role of Transmembrane Domain 6 in Human Serotonin and Norepinephrine Transporters Revealed by Molecular Dynamics Simulation. ACS Chemical Neuroscience, 2018, 9, 1128-1140.	3.5	225
3	Consistent gene signature of schizophrenia identified by a novel feature selection strategy from comprehensive sets of transcriptomic data. Briefings in Bioinformatics, 2020, 21, 1058-1068.	6.5	177
4	ANPELA: analysis and performance assessment of the label-free quantification workflow for metaproteomic studies. Briefings in Bioinformatics, 2020, 21, 621-636.	6.5	151
5	Nucleocapsid mutations R203K/G204R increase the infectivity, fitness, and virulence of SARS-CoV-2. Cell Host and Microbe, 2021, 29, 1788-1801.e6.	11.0	145
6	Clinical trials, progression-speed differentiating features and swiftness rule of the innovative targets of first-in-class drugs. Briefings in Bioinformatics, 2020, 21, 649-662.	6.5	139
7	Computational identification of the binding mechanism of a triple reuptake inhibitor amitifadine for the treatment of major depressive disorder. Physical Chemistry Chemical Physics, 2018, 20, 6606-6616.	2.8	125
8	Performance Evaluation and Online Realization of Data-driven Normalization Methods Used in LC/MS based Untargeted Metabolomics Analysis. Scientific Reports, 2016, 6, 38881.	3.3	117
9	Simultaneous Improvement in the Precision, Accuracy, and Robustness of Label-free Proteome Quantification by Optimizing Data Manipulation Chains*. Molecular and Cellular Proteomics, 2019, 18, 1683-1699.	3.8	113
10	Exploring the Binding Mechanism of Metabotropic Glutamate Receptor 5 Negative Allosteric Modulators in Clinical Trials by Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2018, 9, 1492-1502.	3.5	108
11	Protein functional annotation of simultaneously improved stability, accuracy and false discovery rate achieved by a sequence-based deep learning. Briefings in Bioinformatics, 2020, 21, 1437-1447.	6.5	105
12	Interaction of erucic acid with bovine serum albumin using a multi-spectroscopic method and molecular docking technique. Food Chemistry, 2015, 173, 31-37.	8.2	95
13	ORF8 contributes to cytokine storm during SARS-CoV-2 infection by activating IL-17 pathway. IScience, 2021, 24, 102293.	4.1	94
14	Convolutional neural network-based annotation of bacterial type IV secretion system effectors with enhanced accuracy and reduced false discovery. Briefings in Bioinformatics, 2020, 21, 1825-1836.	6.5	90
15	How Does Chirality Determine the Selective Inhibition of Histone Deacetylase 6? A Lesson from Trichostatin A Enantiomers Based on Molecular Dynamics. ACS Chemical Neuroscience, 2019, 10, 2467-2480.	3.5	86
16	Molecular modeling study on the resistance mechanism of HCV NS3/4A serine protease mutants R155K, A156V and D168A to TMC435. Antiviral Research, 2012, 93, 126-137.	4.1	79
17	Exploring the Molecular Mechanism of Cross-Resistance to HIV-1 Integrase Strand Transfer Inhibitors by Molecular Dynamics Simulation and Residue Interaction Network Analysis. Journal of Chemical Information and Modeling, 2013, 53, 210-222.	5.4	75
18	Discovery of the Consistently Well-Performed Analysis Chain for SWATH-MS Based Pharmacoproteomic Quantification. Frontiers in Pharmacology, 2018, 9, 681.	3.5	69

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19	Identification of the inhibitory mechanism of FDA approved selective serotonin reuptake inhibitors: an insight from molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2016, 18, 3260-3271.	2.8	66
20	Molecular Mechanism for the Allosteric Inhibition of the Human Serotonin Transporter by Antidepressant Escitalopram. ACS Chemical Neuroscience, 2022, 13, 340-351.	3.5	65
21	Differentiating Physicochemical Properties between Addictive and Nonaddictive ADHD Drugs Revealed by Molecular Dynamics Simulation Studies. ACS Chemical Neuroscience, 2017, 8, 1416-1428.	3.5	61
22	SSizer: Determining the Sample Sufficiency for Comparative Biological Study. Journal of Molecular Biology, 2020, 432, 3411-3421.	4.2	60
23	Computational Study on the Drug Resistance Mechanism against HCV NS3/4A Protease Inhibitors Vaniprevir and MK-5172 by the Combination Use of Molecular Dynamics Simulation, Residue Interaction Network, and Substrate Envelope Analysis. Journal of Chemical Information and Modeling, 2014, 54, 621-633.	5.4	59
24	Steroidal alkaloids from Holarrhena antidysenterica as acetylcholinesterase inhibitors and the investigation for structureâ€“activity relationships. Life Sciences, 2012, 90, 929-933.	4.3	57
25	Differentiating physicochemical properties between NDRIs and sNRIs clinically important for the treatment of ADHD. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2766-2777.	2.4	56
26	Structure-Based Discovery of Novel Nonpeptide Inhibitors Targeting SARS-CoV-2 M^{pro}. Journal of Chemical Information and Modeling, 2021, 61, 3917-3926.	5.4	52
27	The Human Kinome Targeted by FDA Approved Multi-Target Drugs and Combination Products: A Comparative Study from the Drug-Target Interaction Network Perspective. PLoS ONE, 2016, 11, e0165737.	2.5	51
28	MMEASE: Online meta-analysis of metabolomic data by enhanced metabolite annotation, marker selection and enrichment analysis. Journal of Proteomics, 2021, 232, 104023.	2.4	50
29	SYNBIP: synthetic binding proteins for research, diagnosis and therapy. Nucleic Acids Research, 2022, 50, D560-D570.	14.5	48
30	A novel bioinformatics approach to identify the consistently well-performing normalization strategy for current metabolomic studies. Briefings in Bioinformatics, 2020, 21, 2142-2152.	6.5	47
31	Exploring the Inhibitory Mechanism of Approved Selective Norepinephrine Reuptake Inhibitors and Reboxetine Enantiomers by Molecular Dynamics Study. Scientific Reports, 2016, 6, 26883.	3.3	46
32	Neferine induces autophagy-dependent cell death in apoptosis-resistant cancers via ryanodine receptor and Ca2+-dependent mechanism. Scientific Reports, 2019, 9, 20034.	3.3	44
33	Spectroscopic and molecular modeling evidence of clozapine binding to human serum albumin at subdomain IIA. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1202-1209.	3.9	42
34	Revealing vilazodone's binding mechanism underlying its partial agonism to the 5-HT_{1A} receptor in the treatment of major depressive disorder. Physical Chemistry Chemical Physics, 2017, 19, 28885-28896.	2.8	41
35	Isolation, characterization and acetylcholinesterase inhibitory activity of alkaloids from roots of Stemona sessilifolia. FÃ¬toterapÃ¬Â¢, 2013, 89, 257-264.	2.2	38
36	(Z)3,4,5,4â€²-trans-tetramethoxystilbene, a new analogue of resveratrol, inhibits gefitinb-resistant non-small cell lung cancer via selectively elevating intracellular calcium level. Scientific Reports, 2015, 5, 16348.	3.3	38

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37	Computational characterization of the selective inhibition of human norepinephrine and serotonin transporters by an escitalopram scaffold. Physical Chemistry Chemical Physics, 2018, 20, 29513-29527.	2.8	37
38	Interaction studies of aristolochic acid I with human serum albumin and the binding site of aristolochic acid I in subdomain IIA. International Journal of Biological Macromolecules, 2011, 49, 343-350.	7.5	36
39	Molecular mechanism of HIVâ€1 integraseâ€“vDNA interactions and strand transfer inhibitor action: A molecular modeling perspective. Journal of Computational Chemistry, 2012, 33, 527-536.	3.3	36
40	Comparison of FDA Approved Kinase Targets to Clinical Trial Ones: Insights from Their System Profiles and Drug-Target Interaction Networks. BioMed Research International, 2016, 2016, 1-9.	1.9	36
41	Molecular modeling and residue interaction network studies on the mechanism of binding and resistance of the HCV NS5B polymerase mutants to VX-222 and ANA598. Antiviral Research, 2014, 104, 40-51.	4.1	35
42	Assessing the Performances of Protein Function Prediction Algorithms from the Perspectives of Identification Accuracy and False Discovery Rate. International Journal of Molecular Sciences, 2018, 19, 183.	4.1	35
43	Genome-wide identification and analysis of the eQTL lncRNAs in multiple sclerosis based on RNA-seq data. Briefings in Bioinformatics, 2020, 21, 1023-1037.	6.5	35
44	Elucidating the tight-binding mechanism of two oral anticoagulants to factor Xa by using induced-fit docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 625-633.	3.5	35
45	Computational design and modeling of nanobodies toward SARSâ€CoVâ€2 receptor binding domain. Chemical Biology and Drug Design, 2021, 98, 1-18.	3.2	35
46	A critical assessment of the feature selection methods used for biomarker discovery in current metaproteomics studies. Briefings in Bioinformatics, 2020, 21, 1378-1390.	6.5	34
47	Understanding the drug resistance mechanism of hepatitis C virus NS3/4A to ITMN-191 due to R155K, A156V, D168A/E mutations: A computational study. Biochimica Et Biophysica Acta - General Subjects, 2012, 1820, 1526-1534.	2.4	33
48	The binding mode of vilazodone in the human serotonin transporter elucidated by ligand docking and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 5132-5144.	2.8	33
49	Identification of novel immuneâ€relevant drug target genes for Alzheimer's Disease by combining ontology inference with network analysis. CNS Neuroscience and Therapeutics, 2018, 24, 1253-1263.	3.9	32
50	MicroRNA-325-3p Facilitates Immune Escape of Mycobacterium tuberculosis through Targeting LNX1 via NEK6 Accumulation to Promote Anti-Apoptotic STAT3 Signaling. MBio, 2020, 11, .	4.1	32
51	Prediction of the binding mode and resistance profile for a dual-target pyrrolyl diketo acid scaffold against HIV-1 integrase and reverse-transcriptase-associated ribonuclease H. Physical Chemistry Chemical Physics, 2018, 20, 23873-23884.	2.8	31
52	Identification of the gene signature reflecting schizophreniaâ€™s etiology by constructing artificial intelligenceâ€based method of enhanced reproducibility. CNS Neuroscience and Therapeutics, 2019, 25, 1054-1063.	3.9	31
53	GIMICA: host genetic and immune factors shaping human microbiota. Nucleic Acids Research, 2021, 49, D715-D722.	14.5	29
54	Determining the Balance Between Drug Efficacy and Safety by the Network and Biological System Profile of Its Therapeutic Target. Frontiers in Pharmacology, 2018, 9, 1245.	3.5	28

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55	Understanding the structural and energetic basis of inhibitor and substrate bound to the full-length NS3/4A: insights from molecular dynamics simulation, binding free energy calculation and network analysis. Molecular BioSystems, 2012, 8, 2753.	2.9	26
56	N-Desmethyldauricine Induces Autophagic Cell Death in Apoptosis-Defective Cells via Ca2+ Mobilization. Frontiers in Pharmacology, 2017, 8, 388.	3.5	26
57	Synthesis and structureâ€“activity relationship of nuciferine derivatives as potential acetylcholinesterase inhibitors. Medicinal Chemistry Research, 2014, 23, 3178-3186.	2.4	25
58	Assessing the Effectiveness of Direct Data Merging Strategy in Long-Term and Large-Scale Pharmacometabonomics. Frontiers in Pharmacology, 2019, 10, 127.	3.5	25
59	Subtype-selective mechanisms of negative allosteric modulators binding to group I metabotropic glutamate receptors. Acta Pharmacologica Sinica, 2021, 42, 1354-1367.	6.1	25
60	Understanding the effect of drug-resistant mutations of HIV-1 intasome on raltegravir action through molecular modeling study. Molecular BioSystems, 2012, 8, 2135.	2.9	24
61	Identification of dual active agents targeting 5-HT1A and SERT by combinatorial virtual screening methods. Bio-Medical Materials and Engineering, 2015, 26, S2233-S2239.	0.6	24
62	Biomarker Discovery for Immunotherapy of Pituitary Adenomas: Enhanced Robustness and Prediction Ability by Modern Computational Tools. International Journal of Molecular Sciences, 2019, 20, 151.	4.1	24
63	Recent Advances and Challenges of the Drugs Acting on Monoamine Transporters. Current Medicinal Chemistry, 2020, 27, 3830-3876.	2.4	24
64	MiRâ€342 controls Mycobacterium tuberculosis susceptibility by modulating inflammation and cell death. EMBO Reports, 2021, 22, e52252.	4.5	22
65	Comparison of computational model and X-ray crystal structure of human serotonin transporter: potential application for the pharmacology of human monoamine transporters. Molecular Simulation, 2017, 43, 1089-1098.	2.0	21
66	Molecular Simulation of Oncostatin M and Receptor (OSMâ€“OSMR) Interaction as a Potential Therapeutic Target for Inflammatory Bowel Disease. Frontiers in Molecular Biosciences, 2020, 7, 29.	3.5	21
67	Computational Study on the Inhibitor Binding Mode and Allosteric Regulation Mechanism in Hepatitis C Virus NS3/4A Protein. PLoS ONE, 2014, 9, e87077.	2.5	19
68	Computational study on the drug resistance mechanism of hepatitis C virus NS5B RNA-dependent RNA polymerase mutants to BMS-791325 by molecular dynamics simulation and binding free energy calculations. Chemometrics and Intelligent Laboratory Systems, 2016, 154, 185-193.	3.5	18
69	Transition State-Based Sialyltransferase Inhibitors: Mimicking Oxocarbenium Ion by Simple Amide. Journal of Medicinal Chemistry, 2017, 60, 2135-2141.	6.4	18
70	Understanding the Polypharmacological Profiles of Triple Reuptake Inhibitors by Molecular Simulation. ACS Chemical Neuroscience, 2021, 12, 2013-2026.	3.5	18
71	Molecular Modeling Study on the Allosteric Inhibition Mechanism of HIV-1 Integrase by LEDGF/p75 Binding Site Inhibitors. PLoS ONE, 2014, 9, e90799.	2.5	16
72	Prediction of GluN2B-CT1290-1310/DAPK1 Interaction by Proteinâ€“Peptide Docking and Molecular Dynamics Simulation. Molecules, 2018, 23, 3018.	3.8	16

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73	Identification of Key Long Non-Coding RNAs in the Pathology of Alzheimerâ€™s Disease and their Functions Based on Genome-Wide Associations Study, Microarray, and RNA-seq Data. Journal of Alzheimer's Disease, 2019, 68, 339-355.	2.6	16
74	What Makes Species Productive of Anti-Cancer Drugs? Clues from Drugsâ€™ Species Origin, Druglikeness, Target and Pathway. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 194-203.	1.7	16
75	Understanding the drug resistance mechanism of hepatitis C virus NS5B to PF-00868554 due to mutations of the 423 site: a computational study. Molecular BioSystems, 2014, 10, 767.	2.9	15
76	Cross-reactivity of two human IL-6 family cytokines OSM and LIF explored by protein-protein docking and molecular dynamics simulation. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129907.	2.4	15
77	Computational Advances in the Label-free Quantification of Cancer Proteomics Data. Current Pharmaceutical Design, 2019, 24, 3842-3858.	1.9	13
78	Identification of Anti-TNFÎ± VNAR Single Domain Antibodies from Whitespotted Bambooshark (Chiloscyllium plagiosum). Marine Drugs, 2022, 20, 307.	4.6	12
79	Virtual screening and experimental validation of eEF2K inhibitors by combining homology modeling, QSAR and molecular docking from FDA approved drugs. New Journal of Chemistry, 2019, 43, 19097-19106.	2.8	9
80	Selective Inhibition of HDAC1 by Macrocyclic Polypeptide for the Treatment of Glioblastoma: A Binding Mechanistic Analysis Based on Molecular Dynamics. Frontiers in Molecular Biosciences, 2020, 7, 41.	3.5	9
81	Copper (Cu²⁺) ion-induced misfolding of tau protein R3 peptide revealed by enhanced molecular dynamics simulation. Physical Chemistry Chemical Physics, 2021, 23, 11717-11726.	2.8	9
82	Integrating the Ribonucleic Acid Sequencing Data From Various Studies for Exploring the Multiple Sclerosis-Related Long Noncoding Ribonucleic Acids and Their Functions. Frontiers in Genetics, 2019, 10, 1136.	2.3	7
83	Cell size prediction of a closed aluminum foam. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 431, 298-305.	5.6	5
84	Phenolic Compounds from Liquidambar formosana Fruits as Monoamine Oxidase Inhibitors. Chemistry of Natural Compounds, 2014, 50, 1118-1119.	0.8	5
85	Insights into conformational regulation of PfMATE transporter from Pyrococcus furiosus induced by alternating protonation state of Asp41 residue: A molecular dynamics simulation study. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 1173-1180.	2.4	5
86	Recent Advances in Computer-aided Antiviral Drug Design Targeting HIV-1 Integrase and Reverse Transcriptase Associated Ribonuclease H. Current Medicinal Chemistry, 2022, 29, 1664-1676.	2.4	3
87	Synthesis, Biological Activity Evaluation and Molecular Modeling Study on the New Isoconessimine Derivatives as Acetylcholinesterase Inhibitors. Chinese Journal of Chemistry, 2013, 31, 1228-1233.	4.9	2
88	Computational study on the inhibition mechanism of a cyclic peptide MaD5 to PfMATE: Insight from molecular dynamics simulation, free energy calculation and dynamical network analysis. Chemometrics and Intelligent Laboratory Systems, 2015, 149, 81-88.	3.5	2
89	Flexible multidentate benzyldiamine derivatives with high affinity for Î²-amyloid in cerebral amyloid angiopathy. Molecular Diversity, 2021, 25, 525-533.	3.9	2
90	Nucleocapsid Mutations R203K/G204R Increase the Infectivity, Fitness and Virulence of SARS-CoV-2. SSRN Electronic Journal, 0, , .	0.4	2

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91	Recent Technological Advances in the Mass Spectrometry-based Nanomedicine Studies: An Insight from Nanoproteomics. Current Pharmaceutical Design, 2019, 25, 1536-1553.	1.9	1