Xuemei Pu

List of Publications by Year in descending order

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65	1,183	394421	454955
papers	citations	19 h-index	30 g-index

66	66	66	1658
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Mechanisms of Diverse Activation Stimulated by Different Biased Agonists for the Î²2-Adrenergic Receptor. Journal of Chemical Information and Modeling, 2022, 62, 5175-5192.	5.4	16
2	Probing Allosteric Regulation Mechanism of W7.35 on Agonist-Induced Activity for Î¼OR by Mutation Simulation. Journal of Chemical Information and Modeling, 2022, 62, 5120-5135.	5.4	6
3	Molecular insights into the allosteric coupling mechanism between an agonist and two different transducers for Î¼-opioid receptors. Physical Chemistry Chemical Physics, 2022, 24, 5282-5293.	2.8	3
4	A Transfer-Learning-Based Deep Convolutional Neural Network for Predicting Leukemia-Related Phosphorylation Sites from Protein Primary Sequences. International Journal of Molecular Sciences, 2022, 23, 1741.	4.1	5
5	An Interpretable Convolutional Neural Network Framework for Analyzing Molecular Dynamics Trajectories: a Case Study on Functional States for G-Protein-Coupled Receptors. Journal of Chemical Information and Modeling, 2022, 62, 1399-1410.	5.4	11
6	A property-oriented adaptive design framework for rapid discovery of energetic molecules based on small-scale labeled datasets. RSC Advances, 2021, 11, 25764-25776.	3.6	2
7	Prediction of Synergistic Drug Combinations for Prostate Cancer by Transcriptomic and Network Characteristics. Frontiers in Pharmacology, 2021, 12, 634097.	3.5	10
8	Coupling complementary strategy to flexible graph neural network for quick discovery of coformer in diverse co-crystal materials. Nature Communications, 2021, 12, 5950.	12.8	37
9	Exploring the Activation Mechanism of a Metabotropic Glutamate Receptor Homodimer via Molecular Dynamics Simulation. ACS Chemical Neuroscience, 2020, 11, 133-145.	3.5	12
10	ExoceRNA atlas: A database of cancer ceRNAs in human blood exosomes. Life Sciences, 2020, 257, 118092.	4.3	6
11	Uncovering the prognostic gene signatures for the improvement of risk stratification in cancers by using deep learning algorithm coupled with wavelet transform. BMC Bioinformatics, 2020, 21, 195.	2.6	4
12	A Novel Detector Based on Convolution Neural Networks for Multiscale SAR Ship Detection in Complex Background. Sensors, 2020, 20, 2547.	3.8	36
13	An Ultraviolet Thermally Activated Delayed Fluorescence OLED with Total External Quantum Efficiency over 9%. Advanced Materials, 2020, 32, e2001248.	21.0	134
14	An effective seven-CpG-based signature to predict survival in renal clear cell carcinoma by integrating DNA methylation and gene expression. Life Sciences, 2020, 243, 117289.	4.3	6
15	Molecular Mechanism Regarding Allosteric Modulation of Ligand Binding and the Impact of Mutations on Dimerization for CCR5 Homodimer. Journal of Chemical Information and Modeling, 2019, 59, 1965-1976.	5.4	15
16	A Novel Convolutional Neural Network Architecture for SAR Target Recognition. Journal of Sensors, 2019, 2019, 1-9.	1.1	19
17	Comparative Analysis for the Performance of Variant Calling Pipelines on Detecting the de novo Mutations in Humans. Frontiers in Pharmacology, 2019, 10, 358.	3.5	12
18	Probing the Druggablility on the Interface of the Proteinâ€“Protein Interaction and Its Allosteric Regulation Mechanism on the Drug Screening for the CXCR4 Homodimer. Frontiers in Pharmacology, 2019, 10, 1310.	3.5	5

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19	Probing the Effects of the Number and Positions of â^'OCH3and â^'CN Substituents on Color Tuning of Ir(III) Complex Derivatives through a Joint Computational and Experimental Study. ChemPhysChem, 2019, 20, 470-481.	2.1	4
20	Use multiscale simulation to explore the effects of the homodimerizations between different conformation states on the activation and allosteric pathway for the Î¼-opioid receptor. Physical Chemistry Chemical Physics, 2018, 20, 13485-13496.	2.8	16
21	Acquiring Highâ€Performance Deepâ€Blue OLED Emitters through an Unexpected Blueshift Colorâ€Tuning Effect Induced by Electronâ€Donating â€OMe Substituents. Chemistry - A European Journal, 2018, 24, 8056-8060.	3.3	38
22	T7 RNA Polymerase Discriminates Correct and Incorrect Nucleoside Triphosphates by Free Energy. Biophysical Journal, 2018, 114, 1755-1761.	0.5	18
23	Using Photocatalytic Oxidation and Analytic Techniques To Remediate Lab Wastewater Containing Methanol. Journal of Chemical Education, 2018, 95, 131-135.	2.3	5
24	Using accelerated molecular dynamics simulation to shed light on the mechanism of activation/deactivation upon mutations for CCR5. RSC Advances, 2018, 8, 37855-37865.	3.6	9
25	Probing the cooperative mechanism of the Î¼â€“Î´ opioid receptor heterodimer by multiscale simulation. Physical Chemistry Chemical Physics, 2018, 20, 29969-29982.	2.8	24
26	The landscape of miRNA-related ceRNA networks for marking different renal cell carcinoma subtypes. Briefings in Bioinformatics, 2018, , .	6.5	5
27	Individually double minimum-distance definition of proteinâ€“RNA binding residues and application to structure-based prediction. Journal of Computer-Aided Molecular Design, 2018, 32, 1363-1373.	2.9	5
28	Shining Light on Molecular Mechanism for Odor-selectivity of CNT-immobilized Olfactory Receptor. Scientific Reports, 2018, 8, 7824.	3.3	9
29	Raman spectroscopy coupled with principal component analysis to quantitatively analyze four crystallographic phases of explosive CL-20. RSC Advances, 2018, 8, 23348-23352.	3.6	21
30	Functional dissection of human targets for KSHV-encoded miRNAs using network analysis. Scientific Reports, 2017, 7, 3159.	3.3	4
31	A sequence-based computational method for prediction of MoRFs. RSC Advances, 2017, 7, 18937-18945.	3.6	8
32	Exploring functions of long noncoding RNAs across multiple cancers through co-expression network. Scientific Reports, 2017, 7, 754.	3.3	41
33	Distinguishing the disease-associated SNPs based on composition frequency analysis. Interdisciplinary Sciences, Computational Life Sciences, 2017, 9, 459-467.	3.6	4
34	Effective prediction of bacterial type IV secreted effectors by combined features of both C-termini and N-termini. Journal of Computer-Aided Molecular Design, 2017, 31, 1029-1038.	2.9	21
35	Structural Features and Ligand Selectivity for 10 Intermediates in the Activation Process of Î²₂-Adrenergic Receptor. ACS Omega, 2017, 2, 8557-8567.	3.5	7
36	Synthesis and Characterization of New Solution-Processable Red Iridium (III) Complexes Based on a Phenylation Strategy. Acta Chimica Sinica, 2017, 75, 367.	1.4	5

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37	A Combination of Chemometrics and Quantum Mechanics Methods Applied to Analysis of Femtosecond Transient Absorption Spectrum of Ortho-Nitroaniline. Scientific Reports, 2016, 6, 19364.	3.3	8
38	Molecular mechanism of carbon nanotube to activate Subtilisin Carlsberg in polar and non-polar organic media. Scientific Reports, 2016, 6, 36838.	3.3	9
39	A facile color-tuning strategy for constructing a library of Ir(<scp>iii</scp>) complexes with fine-tuned phosphorescence from bluish green to red using a synergetic substituent effect of â€“OCH₃ and â€“CN at only the C-ring of C^N ligand. Journal of Materials Chemistry C, 2016, 4, 4269-4277.	5.5	36
40	A facile strategy applied to simultaneous qualitative-detection on multiple components of mixture samples: a joint study of infrared spectroscopy and multi-label algorithms on PBX explosives. RSC Advances, 2016, 6, 4713-4722.	3.6	1
41	Unfolding mechanism of thrombin-binding aptamer revealed by molecular dynamics simulation and Markov State Model. Scientific Reports, 2016, 6, 24065.	3.3	21
42	Exploring the mechanism of F282L mutation-caused constitutive activity of GPCR by a computational study. Physical Chemistry Chemical Physics, 2016, 18, 29412-29422.	2.8	11
43	Use of network model to explore dynamic and allosteric properties of three GPCR homodimers. RSC Advances, 2016, 6, 106327-106339.	3.6	12
44	An effective Ï€-extended squaraine for solution-processed organic solar cells with high efficiency. Journal of Materials Chemistry A, 2016, 4, 18931-18941.	10.3	30
45	Dissecting the regulation rules of cancer-related miRNAs based on network analysis. Scientific Reports, 2016, 6, 34172.	3.3	9
46	Simultaneous determination of multiple components in explosives using ultraviolet spectrophotometry and a partial least squares method. RSC Advances, 2015, 5, 13021-13027.	3.6	16
47	Simultaneous harvesting of triplet excitons in OLEDs by both guest and host materials with an intramolecular charge-transfer feature via tripletâ€“triplet annihilation. Journal of Materials Chemistry C, 2015, 3, 6970-6978.	5.5	20
48	Asymmetrical Squaraines Bearing Fluorine-Substituted Indoline Moieties for High-Performance Solution-Processed Small-Molecule Organic Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 13675-13684.	8.0	39
49	Probing Immobilization Mechanism of alpha-chymotrypsin onto Carbon Nanotube in Organic Media by Molecular Dynamics Simulation. Scientific Reports, 2015, 5, 9297.	3.3	32
50	N,N-Diarylamino end-capping as a new strategy for simultaneously enhancing open-circuit voltage, short-circuit current density and fill factor in small molecule organic solar cells. RSC Advances, 2015, 5, 20724-20733.	3.6	17
51	Self-promoted phthalimide-containing phthalonitrile resins with sluggish curing process and excellent thermal stability. RSC Advances, 2015, 5, 16199-16206.	3.6	69
52	Cyano-substitution on the end-capping group: facile access toward asymmetrical squaraine showing strong dipoleâ€“dipole interactions as a high performance small molecular organic solar cells material. Journal of Materials Chemistry A, 2015, 3, 17704-17712.	10.3	40
53	A consensus subunit-specific model for annotation of substrate specificity for ABC transporters. RSC Advances, 2015, 5, 42009-42019.	3.6	6
54	Exploring the relationship between hub proteins and drug targets based on GO and intrinsic disorder. Computational Biology and Chemistry, 2015, 56, 41-48.	2.3	12

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55	Understanding the conformation transition in the activation pathway of Î²2 adrenergic receptor via a targeted molecular dynamics simulation. Physical Chemistry Chemical Physics, 2015, 17, 2512-2522.	2.8	21
56	Characteristic wavenumbers of Raman spectra reveal the molecular mechanisms of oral leukoplakia and can help to improve the performance of diagnostic models. Analytical Methods, 2015, 7, 590-597.	2.7	1
57	Self-assembled nanopillar arrays by simple spin coating from blending systems comprising PC61BM and conjugated polymers with special structure. RSC Advances, 2014, 4, 24316-24319.	3.6	3
58	Iridium(iii) complexes with enhanced film amorphism as guests for efficient orange solution-processed single-layer PhOLEDs with low efficiency roll-off. Dalton Transactions, 2013, 42, 10559.	3.3	21
59	Effective Identification of Gram-Negative Bacterial Type III Secreted Effectors Using Position-Specific Residue Conservation Profiles. PLoS ONE, 2013, 8, e84439.	2.5	27
60	Synthesis and photovoltaic properties of conjugated copolymers bearing planar acenaphtho[1,2-b]quinoxaline moiety with deep HOMO level. Journal of Materials Science, 2012, 47, 5535-5545.	3.7	22
61	Fine tuning of emission color of iridium(iii) complexes from yellow to red via substituent effect on 2-phenylbenzothiazole ligands: synthesis, photophysical, electrochemical and DFT study. Dalton Transactions, 2011, 40, 7153.	3.3	55
62	A COMPARATIVE STUDY OF META/PARA SUBSTITUTION EFFECTS ON THE HYDROGEN-BONDED COMPLEX OF ANILINE-H2O: OBSERVATIONS FROM COMPUTATION. Journal of Theoretical and Computational Chemistry, 2011, 10, 567-579.	1.8	2
63	Solvent effects on isolated formamide and its monohydrated complex: observations from PCM study. New Journal of Chemistry, 2009, 33, 1709.	2.8	12
64	A sextuple hydrogen bonding molecular duplex bearing 1,8-naphthalimide moieties and polymer light-emitting diode based on it. Journal of Materials Chemistry, 2009, 19, 7753.	6.7	12
65	Substituent effects on the hydrogen-bonded complex of anilineâ€“H2O: a computational study. New Journal of Chemistry, 2008, 32, 1060.	2.8	17