Xianjin Xu

List of Publications by Year in descending order

38 papers	1,000 citations	623734 14 h-index	454955 30 g-index
41 all docs	41 docs citations	41 times ranked	1353 citing authors

#	Article	IF	Citations
1	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	2.6	148
2	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	4.2	131
3	Docking-based inverse virtual screening: methods, applications, and challenges. Biophysics Reports, 2018, 4, 1-16.	0.8	99
4	Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
5	Fully Blind Docking at the Atomic Level for Protein-Peptide Complex Structure Prediction. Structure, 2016, 24, 1842-1853.	3.3	86
6	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	2.6	73
7	MDockPeP: An abâ€initio proteinâ€“peptide docking server. Journal of Computational Chemistry, 2018, 39, 2409-2413.	3.3	59
8	Two-stage electroâ€“mechanical coupling of a KV channel in voltage-dependent activation. Nature Communications, 2020, 11, 676.	12.8	46
9	Proteinâ€“protein docking with binding site patch prediction and networkâ€based terms enhanced combinatorial scoring. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3150-3155.	2.6	31
10	Identification of key residues for protein conformational transition using elastic network model. Journal of Chemical Physics, 2011, 135, 174101.	3.0	22
11	A PIP2 substitute mediates voltage sensor-pore coupling in KCNQ activation. Communications Biology, 2020, 3, 385.	4.4	22
12	Thermal Stability and Unfolding Pathways of Sso7d and its Mutant F31A: Insight from Molecular Dynamics Simulation. Journal of Biomolecular Structure and Dynamics, 2011, 28, 717-727.	3.5	21
13	The interactions and recognition of cyclic peptide mimetics of Tat with HIV-1 TAR RNA: a molecular dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2013, 31, 276-287.	3.5	20
14	Identification of Functionally Key Residues in AMPA Receptor with a Thermodynamic Method. Journal of Physical Chemistry B, 2013, 117, 8689-8696.	2.6	15
15	Improving binding mode and binding affinity predictions of docking by ligand-based search of protein conformations: evaluation in D3R grand challenge 2015. Journal of Computer-Aided Molecular Design, 2017, 31, 689-699.	2.9	15
16	PepPro: A Nonredundant Structure Data Set for Benchmarking Peptideâ€“Protein Computational Docking. Journal of Computational Chemistry, 2020, 41, 362-369.	3.3	13
17	Predicting Proteinâ€“Peptide Complex Structures by Accounting for Peptide Flexibility and the Physicochemical Environment. Journal of Chemical Information and Modeling, 2022, 62, 27-39.	5.4	13
18	Lessons learned from participating in D3R 2016 Grand Challenge 2: compounds targeting the farnesoid X receptor. Journal of Computer-Aided Molecular Design, 2018, 32, 103-111.	2.9	12

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19	Performance of MDockPP in CAPRI rounds 28â€29 and 31â€35 including the prediction of waterâ€mediated interactions. Proteins: Structure, Function and Bioinformatics, 2017, 85, 424-434.	2.6	11
20	Predicting proteinâ€“ligand binding modes for CELPP and GC3: workflows and insight. Journal of Computer-Aided Molecular Design, 2019, 33, 367-374.	2.9	11
21	An Analysis of the Influence of Protein Intrinsic Dynamical Properties on its Thermal Unfolding Behavior. Journal of Biomolecular Structure and Dynamics, 2011, 29, 105-121.	3.5	10
22	Detection of persistent organic pollutants binding modes with androgen receptor ligand binding domain by docking and molecular dynamics. BMC Structural Biology, 2013, 13, 16.	2.3	7
23	Performance of human and server prediction in <scp>CAPRI</scp> rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1110-1120.	2.6	6
24	Modulating the voltage sensor of a cardiac potassium channel shows antiarrhythmic effects. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	6
25	Dissimilar Ligands Bind in a Similar Fashion: A Guide to Ligand Binding-Mode Prediction with Application to CELPP Studies. International Journal of Molecular Sciences, 2021, 22, 12320.	4.1	6
26	SM-TF: A structural database of small molecule-transcription factor complexes. Journal of Computational Chemistry, 2016, 37, 1559-1564.	3.3	4
27	MDockPeP: A Web Server for Blind Prediction of Proteinâ€“Peptide Complex Structures. Methods in Molecular Biology, 2020, 2165, 259-272.	0.9	4
28	A Selective Tether Recruits Activated Response Regulator CheB to Its Chemoreceptor Substrate. MBio, 2021, 12, e0310621.	4.1	4
29	Reverse Virtual Screening on Persistent Organic Pollutants 4,4’-DDE and CB-153. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2013, 29, 2276-2285.	4.9	2
30	The Usage of ACCLUSTER for Peptide Binding Site Prediction. Methods in Molecular Biology, 2017, 1561, 3-9.	0.9	2
31	Inhibition of CK2 Activity by TCDD via binding to ATP-competitive binding site of catalytic subunit: Insight from computational studies. Chemical Research in Chinese Universities, 2013, 29, 299-306.	2.6	1
32	MDockServer: An Efficient Docking Platform for Inverse Virtual Screening. Biophysical Journal, 2018, 114, 56a.	0.5	1
33	CP1 Opens I Ks Channels by Substituting PIP 2. Biophysical Journal, 2017, 112, 110a.	0.5	0
34	Blind Prediction of Protein-Peptide Complex Structures: A Novel Method and a Web Server. Biophysical Journal, 2018, 114, 55a.	0.5	0
35	Coupling between Sensors and the Activation Gate in BK Channels Probed by a Chemical Compound. Biophysical Journal, 2018, 114, 479a.	0.5	0
36	CP1 Is a Potent IKs Channel Activator Which Acts by Substituting Phosphatidylinositol 4,5 Bisphosphate. Biophysical Journal, 2019, 116, 542a-543a.	0.5	0

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37	Two-stage â€œHand-and-Elbowâ€•Gating Mechanism of a KV Channel. Biophysical Journal, 2020, 118, 113a.	0.5	0
38	Coupling between Ca2+ binding and the activation gate opening in BK channels probed by an allosteric activator. Biophysical Journal, 2022, 121, 295a.	0.5	0