Shan Chang

List of Publications by Year in Descending Order

61 papers	746 citations	16 h-index	24 g-index
64 ext. papers	970 ext. citations	4.2 avg, IF	4.01 L-index

#	Paper	IF	Citations
61	Novel natural scaffold as hURAT1 inhibitor identified by 3D-shape-based, docking-based virtual screening approach and biological evaluation. *Bioorganic Chemistry*, **2021**, 117, 105444	5.1	1
60	Clinical recommendations for perioperative immunotherapy-induced adverse events in patients with non-small cell lung cancer. *Thoracic Cancer*, **2021**, 12, 1469-1488	3.2	3
59	Nomogram for predicting the overall survival of the patients with oesophageal signet ring cell carcinoma. *Journal of Thoracic Disease*, **2021**, 13, 1315-1326	2.6	
58	Recent Progress of Deep Learning in Drug Discovery. *Current Pharmaceutical Design*, **2021**, 27, 2088-2096	3.3	1
57	Log odds of positive lymph nodes is a better prognostic factor for oesophageal signet ring cell carcinoma than N stage. *World Journal of Clinical Cases*, **2021**, 9, 24-35	1.6	0
56	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1800-1823	4.2	17
55	Template-based modeling and ab-initio docking using CoDock in CAPRI. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 1100-1109	4.2	2
54	Exploiting Surroundedness and Superpixel cues for salient region detection. *Multimedia Tools and Applications*, **2020**, 79, 10935-10951	2.5	
53	An Overview of Computational Tools of Nucleic Acid Binding Site Prediction for Site-specific Proteins and Nucleases. *Protein and Peptide Letters*, **2020**, 27, 370-384	1.9	0
52	Improvement of Prediction Performance With Conjoint Molecular Fingerprint in Deep Learning. *Frontiers in Pharmacology*, **2020**, 11, 606668	5.6	8
51	Disruption of the EGFR-SQSTM1 interaction by a stapled peptide suppresses lung cancer via activating autophagy and inhibiting EGFR signaling. *Cancer Letters*, **2020**, 474, 23-35	9.9	6
50	Multitask deep networks with grid featurization achieve improved scoring performance for protein-ligand binding. *Chemical Biology and Drug Design*, **2020**, 96, 973-983	2.9	4
49	COVID-19 Docking Server: a meta server for docking small molecules, peptides and antibodies against potential targets of COVID-19. *Bioinformatics*, **2020**, 36, 5109-5111	7.2	78
48	Two- and three-dimensional QSAR studies on hURAT1 inhibitors with flexible linkers: topomer CoMFA and HQSAR. *Molecular Diversity*, **2020**, 24, 141-154	3.1	5
47	Helix-Based RNA Landscape Partition and Alternative Secondary Structure Determination. *ACS Omega*, **2019**, 4, 15407-15413	3.9	1
46	A HTRF based competitive binding assay for screening specific inhibitors of HIV-1 capsid assembly targeting the C-Terminal domain of capsid. *Antiviral Research*, **2019**, 169, 104544	10.8	6
45	Insight into the selective binding mechanism of DNMT1 and DNMT3A inhibitors: a molecular simulation study. *Physical Chemistry Chemical Physics*, **2019**, 21, 12931-12947	3.6	23

44	CoDockPP: A Multistage Approach for Global and Site-Specific Protein-Protein Docking. *Journal of Chemical Information and Modeling*, **2019**, 59, 3556-3564	6.1	15
43	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1200-1221	4.2	58
42	Applications of Molecular Simulation in the Discovery of Antituberculosis Drugs: A Review. *Protein and Peptide Letters*, **2019**, 26, 648-663	1.9	5
41	Probing the Behaviour of Cas1-Cas2 upon Protospacer Binding in CRISPR-Cas Systems using Molecular Dynamics Simulations. *Scientific Reports*, **2019**, 9, 3188	4.9	9
40	Molecular Dynamics Simulations of Wild Type and Mutants of SAPAP in Complexed with Shank3. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	22
39	Inhibition of programmed cell death protein ligand-1 (PD-L1) by benzyl ether derivatives: analyses of conformational change, molecular recognition and binding free energy. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 4801-4812	3.6	7
38	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	5.7	17
37	Benchmark Study Based on 2P2I to Gain Insights into the Discovery of Small-Molecule PPI Inhibitors. *Journal of Physical Chemistry B*, **2018**, 122, 2544-2555	3.4	11
36	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	3.6	21
35	Discovery of Novel Androgen Receptor Ligands by Structure-based Virtual Screening and Bioassays. *Genomics, Proteomics and Bioinformatics*, **2018**, 16, 416-427	6.5	19
34	Exploring the RNA-bound and RNA-free human Argonaute-2 by molecular dynamics simulation method. *Chemical Biology and Drug Design*, **2017**, 90, 753-763	2.9	4
33	Molecular Simulation Studies on the Binding Selectivity of Type-I Inhibitors in the Complexes with ROS1 versus ALK. *Journal of Chemical Information and Modeling*, **2017**, 57, 977-987	6.1	11
32	Unraveling the conformational determinants of LARP7 and 7SK small nuclear RNA by theoretical approaches. *Molecular BioSystems*, **2016**, 12, 2613-21		11
31	Potential Role of the Last Half Repeat in TAL Effectors Revealed by a Molecular Simulation Study. *BioMed Research International*, **2016**, 2016, 8036450	3	1
30	Exploring the molecular basis of RNA recognition by the dimeric RNA-binding protein via molecular simulation methods. *RNA Biology*, **2016**, 13, 1133-1143	4.8	14
29	Molecular dynamics simulations of wild type and mutant of Pin1 peptidyl-prolyl isomerase. *Molecular Simulation*, **2016**, 42, 1281-1291	2	2
28	Molecular dynamics simulation study reveals potential substrate entry path into β-secretase/presenilin-1. *Journal of Structural Biology*, **2015**, 191, 120-9	3.4	27
27	Molecular Dynamics Simulations of Ternary Complexes: Comparisons of LEAFY Protein Binding to Different DNA Motifs. *Journal of Chemical Information and Modeling*, **2015**, 55, 784-94	6.1	11

26	Molecular dynamics simulations of wild type and mutants of botulinum neurotoxin A complexed with synaptic vesicle protein 2C. *Molecular BioSystems*, **2015**, 11, 223-31		16
25	Understanding peptide competitive inhibition of botulinum neurotoxin A binding to SV2 protein via molecular dynamics simulations. *Biopolymers*, **2015**, 103, 597-608	2.2	6
24	Study on Molecular Recognition betweenEuphorbia FactorL713283 and□Tubulin via Molecular Simulation Methods. *Journal of Chemistry*, **2015**, 2015, 1-13	2.3	0
23	Conopeptide Vt3.1 preferentially inhibits BK potassium channels containing □4 subunits via electrostatic interactions. *Journal of Biological Chemistry*, **2014**, 289, 4735-42	5.4	15
22	Molecular dynamics simulations of wild type and mutants of human complement receptor 2 complexed with C3d. *Physical Chemistry Chemical Physics*, **2013**, 15, 1241-51	3.6	44
21	Understanding the folding and stability of a designed WW domain protein with replica exchange molecular dynamics simulations. *Molecular Simulation*, **2013**, 39, 828-836	2	4
20	Study on the interactions between diketo-acid inhibitors and prototype foamy virus integrase-DNA complex via molecular docking and comparative molecular dynamics simulation methods. *Journal of Biomolecular Structure and Dynamics*, **2013**, 31, 734-47	3.6	12
19	Substrate recognition and motion mode analyses of PFV integrase in complex with viral DNA via coarse-grained models. *PLoS ONE*, **2013**, 8, e54929	3.7	9
18	Molecular dynamics simulations of DNA-free and DNA-bound TAL effectors. *PLoS ONE*, **2013**, 8, e76045	3.7	34
17	Network models reveal stability and structural rearrangement of signal recognition particle. *Journal of Biomolecular Structure and Dynamics*, **2012**, 30, 150-9	3.6	2
16	Computational model for protein unfolding simulation. *Physical Review E*, **2011**, 83, 061910	2.4	2
15	Allosteric and transport behavior analyses of a fucose transporter with network models. *Soft Matter*, **2011**, 7, 4661	3.6	11
14	Scoring function based on weighted residue network. *International Journal of Molecular Sciences*, **2011**, 12, 8773-86	6.3	8
13	Study on The Binding Mode and Mobility of HIV-1 Integrase With L708, 906 Inhibitor*. *Progress in Biochemistry and Biophysics*, **2011**, 38, 338-346		3
12	Stability and folding behavior analysis of zinc-finger using simple models. *International Journal of Molecular Sciences*, **2010**, 11, 4014-34	6.3	18
11	Substrate recognition and transport behavior analyses of amino acid antiporter with coarse-grained models. *Molecular BioSystems*, **2010**, 6, 2430-8		26
10	A holistic molecular docking approach for predicting protein-protein complex structure. *Science China Life Sciences*, **2010**, 53, 1152-61	8.5	5
9	Network analysis of protein-protein interaction. *Science Bulletin*, **2010**, 55, 814-822		6

8	Protein-protein docking with binding site patch prediction and network-based terms enhanced combinatorial scoring. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 3150-5	4.2	26
7	Evolving model of amino acid networks. *Physical Review E*, **2008**, 77, 061920	2.4	7
6	Amino acid network and its scoring application in protein-protein docking. *Biophysical Chemistry*, **2008**, 134, 111-8	3.5	18
5	A filter enhanced sampling and combinatorial scoring study for protein docking in CAPRI. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 859-65	4.2	4
4	Construction and application of the weighted amino acid network based on energy. *Physical Review E*, **2007**, 75, 051903	2.4	29
3	Study on the drug resistance and the binding mode of HIV-1 integrase with LCA inhibitor. *Science in China Series B: Chemistry*, **2007**, 50, 665-674		5
2	Complex-type-dependent scoring functions in protein-protein docking. *Biophysical Chemistry*, **2007**, 129, 1-10	3.5	14
1	Scoring Function for the Other-type Protein Complexe. *Acta Physico-chimica Sinica*, **2006**, 22, 622-626		2