Yang Shen

List of Publications by Year
in descending order

48 papers	4,556 citations	218677 26 h-index	265206 42 g-index
58 all docs	58 docs citations	58 times ranked	8279 citing authors

#	Article	IF	Citations
1	Circulating ACE2-expressing extracellular vesicles block broad strains of SARS-CoV-2. Nature Communications, 2022, 13, 405.	12.8	92
2	Bringing Your Own View. , 2022, , .		13
3	Explainable Deep Relational Networks for Predicting Compoundâ€"Protein Affinities and Contacts. Journal of Chemical Information and Modeling, 2021, 61, 46-66.	5.4	30
4	TALE: Transformer-based protein function Annotation with joint sequenceâ€"Label Embedding. Bioinformatics, 2021, 37, 2825-2833.	4.1	52
5	Crowdsourced mapping of unexplored target space of kinase inhibitors. Nature Communications, 2021, 12, 3307.	12.8	41
6	ICAM1 initiates CTC cluster formation and trans-endothelial migration in lung metastasis of breast cancer. Nature Communications, 2021, 12, 4867.	12.8	97
7	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
8	Fold2Seq: A Joint Sequence(1D)-Fold(3D) Embedding-based Generative Model for Protein Design. Proceedings of Machine Learning Research, 2021, 139, 1261-1271.	0.3	1
9	Network-principled deep generative models for designing drug combinations as graph sets. Bioinformatics, 2020, 36, i445-i454.	4.1	24
10	L2-GCN: Layer-Wise and Learned Efficient Training of Graph Convolutional Networks. , 2020, , .		29
11	De Novo Protein Design for Novel Folds Using Guided Conditional Wasserstein Generative Adversarial Networks. Journal of Chemical Information and Modeling, 2020, 60, 5667-5681.	5.4	44
12	Bayesian Active Learning for Optimization and Uncertainty Quantification in Protein Docking. Journal of Chemical Theory and Computation, 2020, 16, 5334-5347.	5.3	12
13	Energyâ€based graph convolutional networks for scoring protein docking models. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1091-1099.	2.6	40
14	Extracellular Domains I and II of cell-surface glycoprotein CD44 mediate its trans-homophilic dimerization and tumor cluster aggregation. Journal of Biological Chemistry, 2020, 295, 2640-2649.	3.4	24
15	A Genetically Encoded, Phageâ€Displayed Cyclicâ€Peptide Library. Angewandte Chemie - International Edition, 2019, 58, 15904-15909.	13.8	64
16	Assessment of blind predictions of the clinical significance of BRCA1 and BRCA2 variants. Human Mutation, 2019, 40, 1546-1556.	2.5	19
17	Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
18	Evaluating the predictions of the protein stability change upon single amino acid substitutions for the FXN CAGI5 challenge. Human Mutation, 2019, 40, 1392-1399.	2.5	16

#	Article	IF	Citations
19	Assessing the performance of in silico methods for predicting the pathogenicity of variants in the gene CHEK2, among Hispanic females with breast cancer. Human Mutation, 2019, 40, 1612-1622.	2.5	8
20	Predicting pathogenicity of missense variants with weakly supervised regression. Human Mutation, 2019, 40, 1579-1592.	2.5	5
21	Engineering a HER2-specific antibodyâ€“drug conjugate to increase lysosomal delivery and therapeutic efficacy. Nature Biotechnology, 2019, 37, 523-526.	17.5	58
22	DeepAffinity: interpretable deep learning of compoundâ€“protein affinity through unified recurrent and convolutional neural networks. Bioinformatics, 2019, 35, 3329-3338.	4.1	279
23	Homophilic CD44 Interactions Mediate Tumor Cell Aggregation and Polyclonal Metastasis in Patient-Derived Breast Cancer Models. Cancer Discovery, 2019, 9, 96-113.	9.4	256
24	Genomic and Molecular Landscape of DNA Damage Repair Deficiency across The Cancer Genome Atlas. Cell Reports, 2018, 23, 239-254.e6.	6.4	801
25	iCFN: an efficient exact algorithm for multistate protein design. Bioinformatics, 2018, 34, i811-i820.	4.1	18
26	G protein-coupled receptors in arthropod vectors: omics and pharmacological approaches to elucidate ligand-receptor interactions and novel organismal functions. Current Opinion in Insect Science, 2018, 29, 12-20.	4.4	28
27	The SERM/SERD bazedoxifene disrupts ESR1 helix 12 to overcome acquired hormone resistance in breast cancer cells. ELife, 2018, 7, .	6.0	72
28	Predicting protein conformational changes for unbound and homology docking: learning from intrinsic and induced flexibility. Proteins: Structure, Function and Bioinformatics, 2017, 85, 544-556.	2.6	12
29	Estrogen receptor alpha somatic mutations Y537S and D538G confer breast cancer endocrine resistance by stabilizing the activating function-2 binding conformation. ELife, 2016, 5, .	6.0	212
30	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
31	Biomedical informatics with optimization and machine learning. Eurasip Journal on Bioinformatics and Systems Biology, 2016, 2017, 4.	1.4	3
32	Identification of YbeY-Protein Interactions Involved in 16S rRNA Maturation and Stress Regulation in Escherichia coli. MBio, 2016, 7, .	4.1	51
33	cNMA: a framework of encounter complex-based normal mode analysis to model conformational changes in protein interactions. Bioinformatics, 2015, 31, i151-i160.	4.1	33
34	Molecular mechanisms and design principles for promiscuous inhibitors to avoid drug resistance: Lessons learned from HIV â€1 protease inhibition. Proteins: Structure, Function and Bioinformatics, 2015, 83, 351-372.	2.6	9
35	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	2.6	50
36	ESR1 ligand-binding domain mutations in hormone-resistant breast cancer. Nature Genetics, 2013, 45, 1439-1445.	21.4	960

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37	Testing the Substrate-Envelope Hypothesis with Designed Pairs of Compounds. ACS Chemical Biology, 2013, 8, 2433-2441.	3.4	33
38	Improved flexible refinement of protein docking in CAPRI rounds 22â€“27. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2129-2136.	2.6	17
39	Overcoming mutation-based resistance to antiandrogens with rational drug design. ELife, 2013, 2, e00499.	6.0	334
40	Charge Optimization Theory for Induced-Fit Ligands. Journal of Chemical Theory and Computation, 2012, 8, 4580-4592.	5.3	8
41	Achieving reliability and high accuracy in automated protein docking: Cluspro, PIPER, SDU, and stability analysis in CAPRI rounds 13â€“19. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3124-3130.	2.6	211
42	Protein Docking by the Underestimation of Free Energy Funnels in the Space of Encounter Complexes. PLoS Computational Biology, 2008, 4, e1000191.	3.2	41
43	SDU: A Semidefinite Programming-Based Underestimation Method for Stochastic Global Optimization in Protein Docking. IEEE Transactions on Automatic Control, 2007, 52, 664-676.	5.7	20
44	Optimizing noisy funnel-like functions on the euclidean group with applications to protein docking. , 2007, , .		2
45	Docking with PIPER and refinement with SDU in rounds 6â€“11 of CAPRI. Proteins: Structure, Function and Bioinformatics, 2007, 69, 734-742.	2.6	12
46	ClusPro: Performance in CAPRI rounds 6â€“11 and the new server. Proteins: Structure, Function and Bioinformatics, 2007, 69, 781-785.	2.6	77
47	Protein-protein docking with reduced potentials by exploiting multi-dimensional energy funnels. , 2006, 2006, 5330-3.		4
48	A Semi-Definite programming-based Underestimation method for global optimization in molecular docking. , 0, , .		4