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	ESR1 ligand-binding domain mutations in hormone-resistant breast cancer. Nature Genetics, 2013, 45, 1439-1445.	21.4	960
2	Genomic and Molecular Landscape of DNA Damage Repair Deficiency across The Cancer Genome Atlas. Cell Reports, 2018, 23, 239-254.e6.	6.4	801
3	Overcoming mutation-based resistance to antiandrogens with rational drug design. ELife, 2013, 2, e00499.	6.0	334
4	DeepAffinity: interpretable deep learning of compoundâ€“protein affinity through unified recurrent and convolutional neural networks. Bioinformatics, 2019, 35, 3329-3338.	4.1	279
5	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
6	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
7	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
8	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
9	Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
10	ICAM1 initiates CTC cluster formation and trans-endothelial migration in lung metastasis of breast cancer. Nature Communications, 2021, 12, 4867.	12.8	97
11	Circulating ACE2-expressing extracellular vesicles block broad strains of SARS-CoV-2. Nature Communications, 2022, 13, 405.	12.8	92
12	ClusPro: Performance in CAPRI rounds 6â€“11 and the new server. Proteins: Structure, Function and Bioinformatics, 2007, 69, 781-785.	2.6	77
13	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
14	The SERM/SERD bazedoxifene disrupts ESR1 helix 12 to overcome acquired hormone resistance in breast cancer cells. ELife, 2018, 7, .	6.0	72
15	A Genetically Encoded, Phageâ€Displayed Cyclicâ€Peptide Library. Angewandte Chemie - International Edition, 2019, 58, 15904-15909.	13.8	64
16	Engineering a HER2-specific antibodyâ€“drug conjugate to increase lysosomal delivery and therapeutic efficacy. Nature Biotechnology, 2019, 37, 523-526.	17.5	58
17	TALE: Transformer-based protein function Annotation with joint sequenceâ€“Label Embedding. Bioinformatics, 2021, 37, 2825-2833.	4.1	52
18	Identification of YbeY-Protein Interactions Involved in 16S rRNA Maturation and Stress Regulation in Escherichia coli. MBio, 2016, 7, .	4.1	51

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19	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	2.6	50
20	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
21	Protein Docking by the Underestimation of Free Energy Funnels in the Space of Encounter Complexes. PLoS Computational Biology, 2008, 4, e1000191.	3.2	41
22	Crowdsourced mapping of unexplored target space of kinase inhibitors. Nature Communications, 2021, 12, 3307.	12.8	41
23	Energyâ€based graph convolutional networks for scoring protein docking models. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1091-1099.	2.6	40
24	Testing the Substrate-Envelope Hypothesis with Designed Pairs of Compounds. ACS Chemical Biology, 2013, 8, 2433-2441.	3.4	33
25	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
26	Explainable Deep Relational Networks for Predicting Compoundâ€“Protein Affinities and Contacts. Journal of Chemical Information and Modeling, 2021, 61, 46-66.	5.4	30
27	L2-GCN: Layer-Wise and Learned Efficient Training of Graph Convolutional Networks. , 2020, , .		29
28	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
29	Network-principled deep generative models for designing drug combinations as graph sets. Bioinformatics, 2020, 36, i445-i454.	4.1	24
30	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
31	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
32	Assessment of blind predictions of the clinical significance of BRCA1 and BRCA2 variants. Human Mutation, 2019, 40, 1546-1556.	2.5	19
33	iCFN: an efficient exact algorithm for multistate protein design. Bioinformatics, 2018, 34, i811-i820.	4.1	18
34	Improved flexible refinement of protein docking in CAPRI rounds 22â€“27. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2129-2136.	2.6	17
35	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
36	Bringing Your Own View. , 2022, , .		13

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37	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
38	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
39	Bayesian Active Learning for Optimization and Uncertainty Quantification in Protein Docking. Journal of Chemical Theory and Computation, 2020, 16, 5334-5347.	5.3	12
40	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
41	Charge Optimization Theory for Induced-Fit Ligands. Journal of Chemical Theory and Computation, 2012, 8, 4580-4592.	5.3	8
42	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
43	Predicting pathogenicity of missense variants with weakly supervised regression. Human Mutation, 2019, 40, 1579-1592.	2.5	5
44	A Semi-Definite programming-based Underestimation method for global optimization in molecular docking. , 0, , .		4
45	Protein-protein docking with reduced potentials by exploiting multi-dimensional energy funnels. , 2006, 2006, 5330-3.		4
46	Biomedical informatics with optimization and machine learning. Eurasip Journal on Bioinformatics and Systems Biology, 2016, 2017, 4.	1.4	3
47	Optimizing noisy funnel-like functions on the euclidean group with applications to protein docking. , 2007, , .		2
48	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