Cunliang Geng

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	DeepRank: a deep learning framework for data mining 3D protein-protein interfaces. Nature Communications, 2021, 12, 7068.	12.8	56
2	iScore: a novel graph kernel-based function for scoring protein–protein docking models. Bioinformatics, 2020, 36, 112-121.	4.1	62
3	An overview of dataâ€driven HADDOCK strategies in CAPRI rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1029-1036.	2.6	11
4	iScore: An MPI supported software for ranking protein–protein docking models based on a random walk graph kernel and support vector machines. SoftwareX, 2020, 11, 100462.	2.6	5
5	The pdb2sql Python Package: Parsing, Manipulation and Analysis of PDB Files Using SQL Queries. Journal of Open Source Software, 2020, 5, 2077.	4.6	7
6	matchms - processing and similarity evaluation of mass spectrometry data Journal of Open Source Software, 2020, 5, 2411.	4.6	48
7	Blind prediction of homo―and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
8	Large-scale prediction of binding affinity in protein–small ligand complexes: the PRODIGY-LIG web server. Bioinformatics, 2019, 35, 1585-1587.	4.1	130
9	iSEE: Interface structure, evolution, and energyâ€based machine learning predictor of binding affinity changes upon mutations. Proteins: Structure, Function and Bioinformatics, 2019, 87, 110-119.	2.6	58
10	Finding the ΔΔ <i>G</i> spot: Are predictors of binding affinity changes upon mutations in protein–protein interactions ready for it?. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1410.	14.6	86
11	Performance of HADDOCK and a simple contact-based protein–ligand binding affinity predictor in the D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 175-185.	2.9	97
12	Information-Driven, Ensemble Flexible Peptide Docking Using HADDOCK. Methods in Molecular Biology, 2017, 1561, 109-138.	0.9	35
13	Exploring the interplay between experimental methods and the performance of predictors of binding affinity change upon mutations in protein complexes. Protein Engineering, Design and Selection, 2016, 29, 291-299.	2.1	26
14	Purification, Cloning, Characterization and Essential Amino Acid Residues Analysis of a New ι-Carrageenase from Cellulophaga sp. QY3. PLoS ONE, 2013, 8, e64666.	2.5	22
15	N-Glycoform Diversity of Cellobiohydrolase I from Penicillium decumbens and Synergism of Nonhydrolytic Glycoform in Cellulose Degradation. Journal of Biological Chemistry, 2012, 287, 15906-15915.	3.4	55
16	How Processive Enzymes Work: the Application of Molecular Dynamics Simulation to Study the Catalytic Mechanism. Scientia Sinica Vitae, 2012, 42, 603-612.	0.3	0