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List of Publications by Year in descending order

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Version: 2024-02-01

50
papers

2,569
citations

218677

26
h-index

206112

48
g-index

69
all docs

69
docs citations

69
times ranked

3718
citing authors

#	ARTICLE	IF	CITATIONS
1	SPEAR: Systematic ProtEin AnnotatoR. <i>Bioinformatics</i> , 2022, 38, 3827-3829.	4.1	1
2	Selective CDK9 Inhibition by Natural Compound Toyocamycin in Cancer Cells. <i>Cancers</i> , 2022, 14, 3340.	3.7	9
3	The NRGTEEN Python package: an extensible toolkit for coarse-grained normal mode analysis of proteins, nucleic acids, small molecules and their complexes. <i>Bioinformatics</i> , 2021, 37, 3369-3371.	4.1	13
4	Repurposing proscillaridin A in combination with decitabine against embryonal rhabdomyosarcoma RD cells. <i>Cancer Chemotherapy and Pharmacology</i> , 2021, 88, 845-856.	2.3	2
5	Modelling conformational state dynamics and its role on infection for SARS-CoV-2 Spike protein variants. <i>PLoS Computational Biology</i> , 2021, 17, e1009286.	3.2	79
6	Applications of the NRGsuite and the Molecular Docking Software FlexAID in Computational Drug Discovery and Design. <i>Methods in Molecular Biology</i> , 2018, 1762, 367-388.	0.9	12
7	A three-way inter-molecular network accounts for the CaV β 1-induced functional modulation of the pore-forming CaV1.2 subunit. <i>Journal of Biological Chemistry</i> , 2018, 293, 7176-7188.	3.4	8
8	Identification of an alternative translation initiation site in the sequence of the commonly used Glutathione S-Transferase tag. <i>Journal of Biotechnology</i> , 2018, 286, 14-16.	3.8	8
9	Functional diversity of TMPRSS6 isoforms and variants expressed in hepatocellular carcinoma cell lines. <i>Scientific Reports</i> , 2018, 8, 12562.	3.3	12
10	Purine analogs targeting the guanine riboswitch as potential antibiotics against <i>Clostridioides difficile</i> . <i>European Journal of Medicinal Chemistry</i> , 2018, 143, 755-768.	5.5	28
11	Modulating the selectivity of matriptase-2 inhibitors with unnatural amino acids. <i>European Journal of Medicinal Chemistry</i> , 2017, 129, 110-123.	5.5	17
12	Applications of Normal Mode Analysis Methods in Computational Protein Design. <i>Methods in Molecular Biology</i> , 2017, 1529, 203-214.	0.9	8
13	Remodeling adipose tissue through in silico modulation of fat storage for the prevention of type 2 diabetes. <i>BMC Systems Biology</i> , 2017, 11, 60.	3.0	6
14	Evolutionary studies of ligand binding sites in proteins. <i>Current Opinion in Structural Biology</i> , 2017, 45, 85-90.	5.7	28
15	Large-scale detection of drug off-targets: hypotheses for drug repurposing and understanding side-effects. <i>BMC Pharmacology & Toxicology</i> , 2017, 18, 18.	2.4	53
16	IsoMIF Finder: online detection of binding site molecular interaction field similarities. <i>Bioinformatics</i> , 2016, 32, 621-623.	4.1	22
17	ENCoM server: exploring protein conformational space and the effect of mutations on protein function and stability. <i>Nucleic Acids Research</i> , 2015, 43, W395-W400.	14.5	151
18	Achievements and challenges in structural bioinformatics and computational biophysics. <i>Bioinformatics</i> , 2015, 31, 146-150.	4.1	24

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19	FlexAID: Revisiting Docking on Non-Native-Complex Structures. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1323-1336.	5.4	54
20	Detection of Binding Site Molecular Interaction Field Similarities. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1600-1615.	5.4	45
21	NRGsuite: a PyMOL plugin to perform docking simulations in real time using FlexAID. <i>Bioinformatics</i> , 2015, 31, 3856-3858.	4.1	66
22	Vibrational entropy differences between mesophile and thermophile proteins and their use in protein engineering. <i>Protein Science</i> , 2015, 24, 474-483.	7.6	21
23	Deep-Sequencing of the Peach Latent Mosaic Viroid Reveals New Aspects of Population Heterogeneity. <i>PLoS ONE</i> , 2014, 9, e87297.	2.5	35
24	A Coarse-Grained Elastic Network Atom Contact Model and Its Use in the Simulation of Protein Dynamics and the Prediction of the Effect of Mutations. <i>PLoS Computational Biology</i> , 2014, 10, e1003569.	3.2	88
25	Analysis of Subpocket Selectivity and Identification of Potent Selective Inhibitors for Matriptase and Matriptase-2. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 10198-10204.	6.4	31
26	A curated <i>C. difficile</i> strain 630 metabolic network: prediction of essential targets and inhibitors. <i>BMC Systems Biology</i> , 2014, 8, 117.	3.0	39
27	The Mode of Action of Recombinant <i>Mycobacterium tuberculosis</i> Shikimate Kinase: Kinetics and Thermodynamics Analyses. <i>PLoS ONE</i> , 2013, 8, e61918.	2.5	15
28	IsoCleft Finder – a web-based tool for the detection and analysis of protein binding-site geometric and chemical similarities. <i>F1000Research</i> , 2013, 2, 117.	1.6	12
29	Kinome Render: a stand-alone and web-accessible tool to annotate the human protein kinome tree. <i>PeerJ</i> , 2013, 1, e126.	2.0	85
30	Side-chain rotamer changes upon ligand binding: common, crucial, correlate with entropy and rearrange hydrogen bonding. <i>Bioinformatics</i> , 2012, 28, i423-i430.	4.1	61
31	StAR-related lipid transfer domain protein 5 binds primary bile acids. <i>Journal of Lipid Research</i> , 2012, 53, 2677-2689.	4.2	33
32	Design and Synthesis of Potent, Selective Inhibitors of Matriptase. <i>ACS Medicinal Chemistry Letters</i> , 2012, 3, 530-534.	2.8	57
33	Structural Chemistry of the Histone Methyltransferases Cofactor Binding Site. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 612-623.	5.4	76
34	The structure of the first representative of Pfam family PF06475 reveals a new fold with possible involvement in glycolipid metabolism. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2010, 66, 1211-1217.	0.7	10
35	Structures of the first representatives of Pfam family PF06938 (DUF1285) reveal a new fold with repeated structural motifs and possible involvement in signal transduction. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2010, 66, 1218-1225.	0.7	8
36	Toll-like receptor stimulation differentially regulates vasoactive intestinal peptide type 2 receptor in macrophages. <i>Journal of Cellular and Molecular Medicine</i> , 2009, 13, 3209-3217.	3.6	18

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37	Structural Analysis of Metal Sites in Proteins: Non-heme Iron Sites as a Case Study. <i>Journal of Molecular Biology</i> , 2009, 388, 356-380.	4.2	48
38	Structure of the Human Protein Kinase MPSK1 Reveals an Atypical Activation Loop Architecture. <i>Structure</i> , 2008, 16, 115-124.	3.3	38
39	Detection of 3D atomic similarities and their use in the discrimination of small molecule protein-binding sites. <i>Bioinformatics</i> , 2008, 24, i105-i111.	4.1	89
40	Analysis of binding site similarity, small-molecule similarity and experimental binding profiles in the human cytosolic sulfotransferase family. <i>Bioinformatics</i> , 2007, 23, e104-e109.	4.1	33
41	Structural and Chemical Profiling of the Human Cytosolic Sulfotransferases. <i>PLoS Biology</i> , 2007, 5, e97.	5.6	187
42	A method for localizing ligand binding pockets in protein structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 479-488.	2.6	181
43	Prediction of Protein Function from Structure: Insights from Methods for the Detection of Local Structural Similarities. <i>BioTechniques</i> , 2005, 38, 847-851.	1.8	29
44	Real spherical harmonic expansion coefficients as 3D shape descriptors for protein binding pocket and ligand comparisons. <i>Bioinformatics</i> , 2005, 21, 2347-2355.	4.1	170
45	Importance of solvent accessibility and contact surfaces in modeling side-chain conformations in proteins. <i>Journal of Computational Chemistry</i> , 2004, 25, 712-724.	3.3	126
46	Protein side-chain rearrangement in regions of point mutations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 50, 272-282.	2.6	31
47	Can a pairwise contact potential stabilize native protein folds against decoys obtained by threading? . , 2000, 38, 134-148.		102
48	Side-chain flexibility in proteins upon ligand binding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 39, 261-268.	2.6	253
49	The collapse transition in the HP model. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1998, 249, 374-379.	2.6	6
50	Toll-like receptor stimulation differentially regulates vasoactive intestinal peptide type 2 receptor in macrophages. <i>Journal of Cellular and Molecular Medicine</i> , 0, 13, 3209-3217.	3.6	14