RafaÃ«l Josef Najmanovich

List of Publications by Year
in descending order

50	2,569	218677	206112
papers	citations	26 h-index	48 g-index

69	69	69	3718
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Side-chain flexibility in proteins upon ligand binding. Proteins: Structure, Function and Bioinformatics, 2000, 39, 261-268.	2.6	253
2	Structural and Chemical Profiling of the Human Cytosolic Sulfotransferases. PLoS Biology, 2007, 5, e97.	5.6	187
3	A method for localizing ligand binding pockets in protein structures. Proteins: Structure, Function and Bioinformatics, 2005, 62, 479-488.	2.6	181
4	Real spherical harmonic expansion coefficients as 3D shape descriptors for protein binding pocket and ligand comparisons. Bioinformatics, 2005, 21, 2347-2355.	4.1	170
5	ENCoM server: exploring protein conformational space and the effect of mutations on protein function and stability. Nucleic Acids Research, 2015, 43, W395-W400.	14.5	151
6	Importance of solvent accessibility and contact surfaces in modeling side-chain conformations in proteins. Journal of Computational Chemistry, 2004, 25, 712-724.	3.3	126
7	Can a pairwise contact potential stabilize native protein folds against decoys obtained by threading?. , 2000, 38, 134-148.		102
8	Detection of 3D atomic similarities and their use in the discrimination of small molecule protein-binding sites. Bioinformatics, 2008, 24, i105-i111.	4.1	89
9	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. PLoS Computational Biology, 2014, 10, e1003569.	3.2	88
10	Kinome Render: a stand-alone and web-accessible tool to annotate the human protein kinome tree. PeerJ, 2013, 1, e126.	2.0	85
11	Modelling conformational state dynamics and its role on infection for SARS-CoV-2 Spike protein variants. PLoS Computational Biology, 2021, 17, e1009286.	3.2	79
12	Structural Chemistry of the Histone Methyltransferases Cofactor Binding Site. Journal of Chemical Information and Modeling, 2011, 51, 612-623.	5.4	76
13	NRGsuite: a PyMOL plugin to perform docking simulations in real time using FlexAID. Bioinformatics, 2015, 31, 3856-3858.	4.1	66
14	Side-chain rotamer changes upon ligand binding: common, crucial, correlate with entropy and rearrange hydrogen bonding. Bioinformatics, 2012, 28, i423-i430.	4.1	61
15	Design and Synthesis of Potent, Selective Inhibitors of Matriptase. ACS Medicinal Chemistry Letters, 2012, 3, 530-534.	2.8	57
16	FlexAID: Revisiting Docking on Non-Native-Complex Structures. Journal of Chemical Information and Modeling, 2015, 55, 1323-1336.	5.4	54
17	Large-scale detection of drug off-targets: hypotheses for drug repurposing and understanding side-effects. BMC Pharmacology & Toxicology, 2017, 18, 18.	2.4	53
18	Structural Analysis of Metal Sites in Proteins: Non-heme Iron Sites as a Case Study. Journal of Molecular Biology, 2009, 388, 356-380.	4.2	48

#	Article	IF	Citations
19	Detection of Binding Site Molecular Interaction Field Similarities. Journal of Chemical Information and Modeling, 2015, 55, 1600-1615.	5.4	45
20	A curated C. difficile strain 630 metabolic network: prediction of essential targets and inhibitors. BMC Systems Biology, 2014, 8, 117.	3.0	39
21	Structure of the Human Protein Kinase MPSK1 Reveals an Atypical Activation Loop Architecture. Structure, 2008, 16, 115-124.	3.3	38
22	Deep-Sequencing of the Peach Latent Mosaic Viroid Reveals New Aspects of Population Heterogeneity. PLoS ONE, 2014, 9, e87297.	2.5	35
23	Analysis of binding site similarity, small-molecule similarity and experimental binding profiles in the human cytosolic sulfotransferase family. Bioinformatics, 2007, 23, e104-e109.	4.1	33
24	StAR-related lipid transfer domain protein 5 binds primary bile acids. Journal of Lipid Research, 2012, 53, 2677-2689.	4.2	33
25	Protein side-chain rearrangement in regions of point mutations. Proteins: Structure, Function and Bioinformatics, 2002, 50, 272-282.	2.6	31
26	Analysis of Subpocket Selectivity and Identification of Potent Selective Inhibitors for Matriptase and Matriptase-2. Journal of Medicinal Chemistry, 2014, 57, 10198-10204.	6.4	31
27	Prediction of Protein Function from Structure: Insights from Methods for the Detection of Local Structural Similarities. BioTechniques, 2005, 38, 847-851.	1.8	29
28	Evolutionary studies of ligand binding sites in proteins. Current Opinion in Structural Biology, 2017, 45, 85-90.	5.7	28
29	Purine analogs targeting the guanine riboswitch as potential antibiotics against Clostridioides difficile. European Journal of Medicinal Chemistry, 2018, 143, 755-768.	5.5	28
30	Achievements and challenges in structural bioinformatics and computational biophysics. Bioinformatics, 2015, 31, 146-150.	4.1	24
31	IsoMIF Finder: online detection of binding site molecular interaction field similarities. Bioinformatics, 2016, 32, 621-623.	4.1	22
32	Vibrational entropy differences between mesophile and thermophile proteins and their use in protein engineering. Protein Science, 2015, 24, 474-483.	7.6	21
33	Toll-like receptor stimulation differentially regulates vasoactive intestinal peptide type 2 receptor in macrophages. Journal of Cellular and Molecular Medicine, 2009, 13, 3209-3217.	3.6	18
34	Modulating the selectivity of matriptase-2 inhibitors with unnatural amino acids. European Journal of Medicinal Chemistry, 2017, 129, 110-123.	5.5	17
35	The Mode of Action of Recombinant Mycobacterium tuberculosis Shikimate Kinase: Kinetics and Thermodynamics Analyses. PLoS ONE, 2013, 8, e61918.	2.5	15
36	Toll-like receptor stimulation differentially regulates vasoactive intestinal peptide type 2 receptor in macrophages. Journal of Cellular and Molecular Medicine, 0, 13, 3209-3217.	3.6	14

#	Article	IF	Citations
37	The NRGTEN Python package: an extensible toolkit for coarse-grained normal mode analysis of proteins, nucleic acids, small molecules and their complexes. Bioinformatics, 2021, 37, 3369-3371.	4.1	13
38	Applications of the NRGsuite and the Molecular Docking Software FlexAID in Computational Drug Discovery and Design. Methods in Molecular Biology, 2018, 1762, 367-388.	0.9	12
39	Functional diversity of TMPRSS6 isoforms and variants expressed in hepatocellular carcinoma cell lines. Scientific Reports, 2018, 8, 12562.	3.3	12
40	IsoCleft Finder â€“ a web-based tool for the detection and analysis of protein binding-site geometric and chemical similarities. F1000Research, 2013, 2, 117.	1.6	12
41	The structure of the first representative of Pfam family PF06475 reveals a new fold with possible involvement in glycolipid metabolism. Acta Crystallographica Section F: Structural Biology Communications, 2010, 66, 1211-1217.	0.7	10
42	Selective CDK9 Inhibition by Natural Compound Toyocamycin in Cancer Cells. Cancers, 2022, 14, 3340.	3.7	9
43	Structures of the first representatives of Pfam family PF06938 (DUF1285) reveal a new fold with repeated structural motifs and possible involvement in signal transduction. Acta Crystallographica Section F: Structural Biology Communications, 2010, 66, 1218-1225.	0.7	8
44	Applications of Normal Mode Analysis Methods in Computational Protein Design. Methods in Molecular Biology, 2017, 1529, 203-214.	0.9	8
45	A three-way inter-molecular network accounts for the CaVÎ±2Î´1-induced functional modulation of the pore-forming CaV1.2 subunit. Journal of Biological Chemistry, 2018, 293, 7176-7188.	3.4	8
46	Identification of an alternative translation initiation site in the sequence of the commonly used Glutathione S-Transferase tag. Journal of Biotechnology, 2018, 286, 14-16.	3.8	8
47	The collapse transition in the HP model. Physica A: Statistical Mechanics and Its Applications, 1998, 249, 374-379.	2.6	6
48	Remodeling adipose tissue through in silico modulation of fat storage for the prevention of type 2 diabetes. BMC Systems Biology, 2017, 11, 60.	3.0	6
49	Repurposing proscillaridin A in combination with decitabine against embryonal rhabdomyosarcoma RD cells. Cancer Chemotherapy and Pharmacology, 2021, 88, 845-856.	2.3	2
50	SPEAR: Systematic ProtEin AnnotatoR. Bioinformatics, 2022, 38, 3827-3829.	4.1	1