Dominik Gront

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3477600/publications.pdf

Version: 2024-02-01

56	2,316	393982	233125
papers	citations	19 h-index	45 g-index

58	58	58	2731
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Coarse-Grained Protein Models and Their Applications. Chemical Reviews, 2016, 116, 7898-7936.	23.0	721
2	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	9.0	513
3	Generalized Fragment Picking in Rosetta: Design, Protocols and Applications. PLoS ONE, 2011, 6, e23294.	1.1	172
4	Backbone building from quadrilaterals: A fast and accurate algorithm for protein backbone reconstruction from alpha carbon coordinates. Journal of Computational Chemistry, 2007, 28, 1593-1597.	1.5	102
5	Comparison of three Monte Carlo conformational search strategies for a proteinlike homopolymer model: Folding thermodynamics and identification of low-energy structures. Journal of Chemical Physics, 2000, 113, 5065.	1.2	66
6	Towards the high-resolution protein structure prediction. Fast refinement of reduced models with all-atom force field. BMC Structural Biology, 2007, 7, 43.	2.3	45
7	BioShell–a package of tools for structural biology computations. Bioinformatics, 2006, 22, 621-622.	1.8	44
8	Utility library for structural bioinformatics. Bioinformatics, 2008, 24, 584-585.	1.8	38
9	Type II restriction endonuclease R.Eco29kI is a member of the GIY-YIG nuclease superfamily. BMC Structural Biology, 2007, 7, 48.	2.3	32
10	Optimization of protein models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 479-493.	6.2	32
11	From Coarse-Grained to Atomic-Level Characterization of Protein Dynamics: Transition State for the Folding of B Domain of Protein A. Journal of Physical Chemistry B, 2012, 116, 7026-7032.	1.2	31
12	HCPM–program for hierarchical clustering of protein models. Bioinformatics, 2005, 21, 3179-3180.	1.8	30
13	A new combination of replica exchange Monte Carlo and histogram analysis for protein folding and thermodynamics. Journal of Chemical Physics, 2001, 115, 1569-1574.	1.2	29
14	Better together: Elements of successful scientific software development in a distributed collaborative community. PLoS Computational Biology, 2020, 16, e1007507.	1.5	27
15	Efficient scheme for optimization of parallel tempering Monte Carlo method. Journal of Physics Condensed Matter, 2007, 19, 036225.	0.7	25
16	Denatured proteins and early folding intermediates simulated in a reduced conformational space.. Acta Biochimica Polonica, 2019, 53, 131-143.	0.3	25
17	Combining Coarse-Grained Protein Models with Replica-Exchange All-Atom Molecular Dynamics. International Journal of Molecular Sciences, 2013, 14, 9893-9905.	1.8	22
18	A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition. Biopolymers, 2003, 69, 399-405.	1.2	21

#	Article	IF	Citations
19	Exploring protein energy landscapes with hierarchical clustering. International Journal of Quantum Chemistry, 2005, 105, 826-830.	1.0	21
20	Biofunctionalisation of p-doped silicon with cytochrome c₅₅₃minimises charge recombination and enhances photovoltaic performance of the all-solid-state photosystem I-based biophotoelectrode. RSC Advances, 2017, 7, 47854-47866.	1.7	21
21	More P450s Are Involved in Secondary Metabolite Biosynthesis in Streptomyces Compared to Bacillus, Cyanobacteria, and Mycobacterium. International Journal of Molecular Sciences, 2020, 21, 4814.	1.8	20
22	SURPASS Low-Resolution Coarse-Grained Protein Modeling. Journal of Chemical Theory and Computation, 2017, 13, 5766-5779.	2.3	18
23	BioShell-Threading: versatile Monte Carlo package for protein 3D threading. BMC Bioinformatics, 2014, 15, 22.	1.2	17
24	In silico analysis of cytochrome P450 monooxygenases in chronic granulomatous infectious fungus Sporothrix schenckii: Special focus on CYP51. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 166-177.	1.1	17
25	Contrasting Health Effects of Bacteroidetes and Firmicutes Lies in Their Genomes: Analysis of P450s, Ferredoxins, and Secondary Metabolite Clusters. International Journal of Molecular Sciences, 2022, 23, 5057.	1.8	17
26	Comparative modeling without implicit sequence alignments. Bioinformatics, 2007, 23, 2522-2527.	1.8	16
27	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	5.8	16
28	The crystal structure of the AF2331 protein from Archaeoglobus fulgidus DSM 4304 forms an unusual interdigitated dimer with a new type of Î± + Î² fold. Protein Science, 2009, 18, 2410-2419.	3.1	11
29	Practical Considerations for Atomistic Structure Modeling with Cryo-EM Maps. Journal of Chemical Information and Modeling, 2020, 60, 2436-2442.	2.5	11
30	In Silico Analysis of P450s and Their Role in Secondary Metabolism in the Bacterial Class Gammaproteobacteria. Molecules, 2021, 26, 1538.	1.7	11
31	BioShell Threader: protein homology detection based on sequence profiles and secondary structure profiles. Nucleic Acids Research, 2012, 40, W257-W262.	6.5	10
32	Assessing the accuracy of template-based structure prediction metaservers by comparison with structural genomics structures. Journal of Structural and Functional Genomics, 2012, 13, 213-225.	1.2	10
33	Comparison of Î±-Helix and Î²-Sheet Structure Adaptation to a Quantum Dot Geometry: Toward the Identification of an Optimal Motif for a Protein Nanoparticle Cover. ACS Omega, 2019, 4, 13086-13099.	1.6	10
34	Denatured proteins and early folding intermediates simulated in a reduced conformational space. Acta Biochimica Polonica, 2006, 53, 131-44.	0.3	10
35	Coarse-Grained Modeling of the Interplay between Secondary Structure Propensities and Protein Fold Assembly. Journal of Chemical Theory and Computation, 2018, 14, 2277-2287.	2.3	9
36	Ancient Bacterial Class Alphaproteobacteria Cytochrome P450 Monooxygenases Can Be Found in Other Bacterial Species. International Journal of Molecular Sciences, 2021, 22, 5542.	1.8	9

#	Article	IF	Citations
37	Diversification of Ferredoxins across Living Organisms. Current Issues in Molecular Biology, 2021, 43, 1374-1390.	1.0	9
38	A new approach to prediction of short-range conformational propensities in proteins. Bioinformatics, 2005, 21, 981-987.	1.8	8
39	Assessing Uncertainty in the Polish Agricultural Greenhouse Gas Emission Inventory Using Monte Carlo Simulation. Outlook on Agriculture, 2014, 43, 61-65.	1.8	8
40	Improving thermal stability of thermophilic l -threonine aldolase from Thermotoga maritima. Journal of Biotechnology, 2015, 199, 69-76.	1.9	8
41	An Unprecedented Number of Cytochrome P450s Are Involved in Secondary Metabolism in Salinispora Species. Microorganisms, 2022, 10, 871.	1.6	8
42	BioShell 3.0: Library for Processing Structural Biology Data. Biomolecules, 2020, 10, 461.	1.8	7
43	Lifestyles Shape the Cytochrome P450 Repertoire of the Bacterial Phylum Proteobacteria. International Journal of Molecular Sciences, 2022, 23, 5821.	1.8	7
44	VisuaLife: library for interactive visualization in rich web applications. Bioinformatics, 2021, 37, 3662-3663.	1.8	6
45	Optimization of Profile-to-Profile Alignment Parameters for One-Dimensional Threading. Journal of Computational Biology, 2012, 19, 879-886.	0.8	4
46	In Silico Structural Modeling and Analysis of Interactions of Tremellomycetes Cytochrome P450 Monooxygenases CYP51s with Substrates and Azoles. International Journal of Molecular Sciences, 2021, 22, 7811.	1.8	4
47	Protein structure prediction by tempering spatial constraints. Journal of Computer-Aided Molecular Design, 2005, 19, 603-608.	1.3	3
48	T-Pile a package for thermodynamic calculations for biomolecules. Bioinformatics, 2007, 23, 1840-1842.	1.8	3
49	Protein Structure Prediction Using Coarse-Grained Models. Springer Series on Bio- and Neurosystems, 2019, , 27-59.	0.2	3
50	Parallel Implementation of a Sequential Markov Chain in Monte Carlo Simulations of Physical Systems with Pairwise Interactions. Journal of Chemical Theory and Computation, 2019, 15, 2797-2806.	2.3	2
51	Coarse-Grained Protein Models in Structure Prediction. Springer Series in Bio-/neuroinformatics, 2014, , 25-53.	0.1	1
52	Automated Protein Secondary Structure Assignment from CÎ± Positions Using Neural Networks. Biomolecules, 2022, 12, 841.	1.8	1
53	Fast and accurate methods for predicting short-range constraints in protein models. Journal of Computer-Aided Molecular Design, 2008, 22, 783-788.	1.3	0
54	De Novo Protein Structure Determination from Incomplete Experimental Data. Biophysical Journal, 2013, 104, 228a.	0.2	0

#	Article	IF	Citations
55	Mutation goals in the vitamin D receptor predicted by computational methods. Journal of Steroid Biochemistry and Molecular Biology, 2018, 183, 210-220.	1.2	0
56	Clustering as a supporting tool for structural drug design. Acta Poloniae Pharmaceutica, 2006, 63, 436-8.	0.3	0