

# Dominik Gront

## List of Publications by Year in descending order

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

Version: 2024-02-01

56  
papers

2,316  
citations

394421

19  
h-index

233421

45  
g-index

58  
all docs

58  
docs citations

58  
times ranked

2731  
citing authors

#	ARTICLE	IF	CITATIONS
1	Coarse-Grained Protein Models and Their Applications. <i>Chemical Reviews</i> , 2016, 116, 7898-7936.	47.7	721
2	Macromolecular modeling and design in Rosetta: recent methods and frameworks. <i>Nature Methods</i> , 2020, 17, 665-680.	19.0	513
3	Generalized Fragment Picking in Rosetta: Design, Protocols and Applications. <i>PLoS ONE</i> , 2011, 6, e23294.	2.5	172
4	Backbone building from quadrilaterals: A fast and accurate algorithm for protein backbone reconstruction from alpha carbon coordinates. <i>Journal of Computational Chemistry</i> , 2007, 28, 1593-1597.	3.3	102
5	Comparison of three Monte Carlo conformational search strategies for a proteinlike homopolymer model: Folding thermodynamics and identification of low-energy structures. <i>Journal of Chemical Physics</i> , 2000, 113, 5065.	3.0	66
6	Towards the high-resolution protein structure prediction. Fast refinement of reduced models with all-atom force field. <i>BMC Structural Biology</i> , 2007, 7, 43.	2.3	45
7	BioShell—a package of tools for structural biology computations. <i>Bioinformatics</i> , 2006, 22, 621-622.	4.1	44
8	Utility library for structural bioinformatics. <i>Bioinformatics</i> , 2008, 24, 584-585.	4.1	38
9	Type II restriction endonuclease R.Eco29kl is a member of the GIY-YIG nuclease superfamily. <i>BMC Structural Biology</i> , 2007, 7, 48.	2.3	32
10	Optimization of protein models. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 479-493.	14.6	32
11	From Coarse-Grained to Atomic-Level Characterization of Protein Dynamics: Transition State for the Folding of B Domain of Protein A. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7026-7032.	2.6	31
12	HCPM—program for hierarchical clustering of protein models. <i>Bioinformatics</i> , 2005, 21, 3179-3180.	4.1	30
13	A new combination of replica exchange Monte Carlo and histogram analysis for protein folding and thermodynamics. <i>Journal of Chemical Physics</i> , 2001, 115, 1569-1574.	3.0	29
14	Better together: Elements of successful scientific software development in a distributed collaborative community. <i>PLoS Computational Biology</i> , 2020, 16, e1007507.	3.2	27
15	Efficient scheme for optimization of parallel tempering Monte Carlo method. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 036225.	1.8	25
16	Denatured proteins and early folding intermediates simulated in a reduced conformational space.. <i>Acta Biochimica Polonica</i> , 2019, 53, 131-143.	0.5	25
17	Combining Coarse-Grained Protein Models with Replica-Exchange All-Atom Molecular Dynamics. <i>International Journal of Molecular Sciences</i> , 2013, 14, 9893-9905.	4.1	22
18	A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition. <i>Biopolymers</i> , 2003, 69, 399-405.	2.4	21

#	ARTICLE	IF	CITATIONS
19	Exploring protein energy landscapes with hierarchical clustering. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 826-830.	2.0	21
20	Biofunctionalisation of p-doped silicon with cytochrome c <sub>553</sub> minimises charge recombination and enhances photovoltaic performance of the all-solid-state photosystem I-based biophotocathode. <i>RSC Advances</i> , 2017, 7, 47854-47866.	3.6	21
21	More P450s Are Involved in Secondary Metabolite Biosynthesis in <i>Streptomyces</i> Compared to <i>Bacillus</i> , <i>Cyanobacteria</i> , and <i>Mycobacterium</i> . <i>International Journal of Molecular Sciences</i> , 2020, 21, 4814.	4.1	20
22	SURPASS Low-Resolution Coarse-Grained Protein Modeling. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5766-5779.	5.3	18
23	BioShell-Threading: versatile Monte Carlo package for protein 3D threading. <i>BMC Bioinformatics</i> , 2014, 15, 22.	2.6	17
24	In silico analysis of cytochrome P450 monooxygenases in chronic granulomatous infectious fungus <i>Sporothrix schenckii</i> : Special focus on CYP51. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2018, 1866, 166-177.	2.3	17
25	Contrasting Health Effects of Bacteroidetes and Firmicutes Lies in Their Genomes: Analysis of P450s, Ferredoxins, and Secondary Metabolite Clusters. <i>International Journal of Molecular Sciences</i> , 2022, 23, 5057.	4.1	17
26	Comparative modeling without implicit sequence alignments. <i>Bioinformatics</i> , 2007, 23, 2522-2527.	4.1	16
27	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. <i>Nature Communications</i> , 2021, 12, 6947.	12.8	16
28	The crystal structure of the AF2331 protein from <i>Archaeoglobus fulgidus</i> DSM 4304 forms an unusual interdigitated dimer with a new type of $\alpha + \beta^2$ fold. <i>Protein Science</i> , 2009, 18, 2410-2419.	7.6	11
29	Practical Considerations for Atomistic Structure Modeling with Cryo-EM Maps. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2436-2442.	5.4	11
30	In Silico Analysis of P450s and Their Role in Secondary Metabolism in the Bacterial Class Gammaproteobacteria. <i>Molecules</i> , 2021, 26, 1538.	3.8	11
31	BioShell Threader: protein homology detection based on sequence profiles and secondary structure profiles. <i>Nucleic Acids Research</i> , 2012, 40, W257-W262.	14.5	10
32	Assessing the accuracy of template-based structure prediction metaservers by comparison with structural genomics structures. <i>Journal of Structural and Functional Genomics</i> , 2012, 13, 213-225.	1.2	10
33	Comparison of $\alpha$ -Helix and $\beta$ -Sheet Structure Adaptation to a Quantum Dot Geometry: Toward the Identification of an Optimal Motif for a Protein Nanoparticle Cover. <i>ACS Omega</i> , 2019, 4, 13086-13099.	3.5	10
34	Denatured proteins and early folding intermediates simulated in a reduced conformational space. <i>Acta Biochimica Polonica</i> , 2006, 53, 131-44.	0.5	10
35	Coarse-Grained Modeling of the Interplay between Secondary Structure Propensities and Protein Fold Assembly. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2277-2287.	5.3	9
36	Ancient Bacterial Class Alphaproteobacteria Cytochrome P450 Monooxygenases Can Be Found in Other Bacterial Species. <i>International Journal of Molecular Sciences</i> , 2021, 22, 5542.	4.1	9

#	ARTICLE	IF	CITATIONS
37	Diversification of Ferredoxins across Living Organisms. <i>Current Issues in Molecular Biology</i> , 2021, 43, 1374-1390.	2.4	9
38	A new approach to prediction of short-range conformational propensities in proteins. <i>Bioinformatics</i> , 2005, 21, 981-987.	4.1	8
39	Assessing Uncertainty in the Polish Agricultural Greenhouse Gas Emission Inventory Using Monte Carlo Simulation. <i>Outlook on Agriculture</i> , 2014, 43, 61-65.	3.4	8
40	Improving thermal stability of thermophilic l -threonine aldolase from <i>Thermotoga maritima</i> . <i>Journal of Biotechnology</i> , 2015, 199, 69-76.	3.8	8
41	An Unprecedented Number of Cytochrome P450s Are Involved in Secondary Metabolism in <i>Salinispora</i> Species. <i>Microorganisms</i> , 2022, 10, 871.	3.6	8
42	BioShell 3.0: Library for Processing Structural Biology Data. <i>Biomolecules</i> , 2020, 10, 461.	4.0	7
43	Lifestyles Shape the Cytochrome P450 Repertoire of the Bacterial Phylum Proteobacteria. <i>International Journal of Molecular Sciences</i> , 2022, 23, 5821.	4.1	7
44	VisuaLife: library for interactive visualization in rich web applications. <i>Bioinformatics</i> , 2021, 37, 3662-3663.	4.1	6
45	Optimization of Profile-to-Profile Alignment Parameters for One-Dimensional Threading. <i>Journal of Computational Biology</i> , 2012, 19, 879-886.	1.6	4
46	In Silico Structural Modeling and Analysis of Interactions of Tremellomycetes Cytochrome P450 Monooxygenases CYP51s with Substrates and Azoles. <i>International Journal of Molecular Sciences</i> , 2021, 22, 7811.	4.1	4
47	Protein structure prediction by tempering spatial constraints. <i>Journal of Computer-Aided Molecular Design</i> , 2005, 19, 603-608.	2.9	3
48	T-Pile a package for thermodynamic calculations for biomolecules. <i>Bioinformatics</i> , 2007, 23, 1840-1842.	4.1	3
49	Protein Structure Prediction Using Coarse-Grained Models. <i>Springer Series on Bio- and Neurosystems</i> , 2019, , 27-59.	0.2	3
50	Parallel Implementation of a Sequential Markov Chain in Monte Carlo Simulations of Physical Systems with Pairwise Interactions. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2797-2806.	5.3	2
51	Coarse-Grained Protein Models in Structure Prediction. <i>Springer Series in Bio-/neuroinformatics</i> , 2014, , 25-53.	0.1	1
52	Automated Protein Secondary Structure Assignment from C $\alpha$ Positions Using Neural Networks. <i>Biomolecules</i> , 2022, 12, 841.	4.0	1
53	Fast and accurate methods for predicting short-range constraints in protein models. <i>Journal of Computer-Aided Molecular Design</i> , 2008, 22, 783-788.	2.9	0
54	De Novo Protein Structure Determination from Incomplete Experimental Data. <i>Biophysical Journal</i> , 2013, 104, 228a.	0.5	0

#	ARTICLE	IF	CITATIONS
55	Mutation goals in the vitamin D receptor predicted by computational methods. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2018, 183, 210-220.	2.5	0
56	Clustering as a supporting tool for structural drug design. <i>Acta Poloniae Pharmaceutica</i> , 2006, 63, 436-8.	0.1	0