# Dominik Gront

## List of Publications by Year
## in descending order

| 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 | An Unprecedented Number of Cytochrome P450s Are Involved in Secondary Metabolism in Salinispora Species. Microorganisms, 2022, 10, 871. | 3.6 | 8 |
| 2 | 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. | 4.1 | 17 |
| 3 | Lifestyles Shape the Cytochrome P450 Repertoire of the Bacterial Phylum Proteobacteria. International Journal of Molecular Sciences, 2022, 23, 5821. | 4.1 | 7 |
| 4 | Automated Protein Secondary Structure Assignment from Cα Positions Using Neural Networks. Biomolecules, 2022, 12, 841. | 4.0 | 1 |
| 5 | In Silico Analysis of P450s and Their Role in Secondary Metabolism in the Bacterial Class Gammaproteobacteria. Molecules, 2021, 26, 1538. | 3.8 | 11 |
| 6 | Ancient Bacterial Class Alphaproteobacteria Cytochrome P450 Monooxygenases Can Be Found in Other Bacterial Species. International Journal of Molecular Sciences, 2021, 22, 5542. | 4.1 | 9 |
| 7 | VisuaLife: library for interactive visualization in rich web applications. Bioinformatics, 2021, 37, 3662-3663. | 4.1 | 6 |
| 8 | 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. | 4.1 | 4 |
| 9 | Diversification of Ferredoxins across Living Organisms. Current Issues in Molecular Biology, 2021, 43, 1374-1390. | 2.4 | 9 |
| 10 | Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947. | 12.8 | 16 |
| 11 | More P450s Are Involved in Secondary Metabolite Biosynthesis in Streptomyces Compared to Bacillus, Cyanobacteria, and Mycobacterium. International Journal of Molecular Sciences, 2020, 21, 4814. | 4.1 | 20 |
| 12 | Better together: Elements of successful scientific software development in a distributed collaborative community. PLoS Computational Biology, 2020, 16, e1007507. | 3.2 | 27 |
| 13 | Practical Considerations for Atomistic Structure Modeling with Cryo-EM Maps. Journal of Chemical Information and Modeling, 2020, 60, 2436-2442. | 5.4 | 11 |
| 14 | Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680. | 19.0 | 513 |
| 15 | BioShell 3.0: Library for Processing Structural Biology Data. Biomolecules, 2020, 10, 461. | 4.0 | 7 |
| 16 | Comparison of α-Helix and β-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. | 3.5 | 10 |
| 17 | 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. | 5.3 | 2 |
| 18 | Protein Structure Prediction Using Coarse-Grained Models. Springer Series on Bio- and Neurosystems, 2019, , 27-59. | 0.2 | 3 |

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|---|---------|-----|-----------|
| 19 | Denatured proteins and early folding intermediates simulated in a reduced conformational space.. Acta Biochimica Polonica, 2019, 53, 131-143. | 0.5 | 25 |
| 20 | Coarse-Grained Modeling of the Interplay between Secondary Structure Propensities and Protein Fold Assembly. Journal of Chemical Theory and Computation, 2018, 14, 2277-2287. | 5.3 | 9 |
| 21 | 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. | 2.3 | 17 |
| 22 | Mutation goals in the vitamin D receptor predicted by computational methods. Journal of Steroid Biochemistry and Molecular Biology, 2018, 183, 210-220. | 2.5 | 0 |
| 23 | SURPASS Low-Resolution Coarse-Grained Protein Modeling. Journal of Chemical Theory and Computation, 2017, 13, 5766-5779. | 5.3 | 18 |
| 24 | Biofunctionalisation of p-doped silicon with cytochrome c$_{553}$ minimises charge recombination and enhances photovoltaic performance of the all-solid-state photosystem I-based biophotoelectrode. RSC Advances, 2017, 7, 47854-47866. | 3.6 | 21 |
| 25 | Coarse-Grained Protein Models and Their Applications. Chemical Reviews, 2016, 116, 7898-7936. | 47.7 | 721 |
| 26 | Improving thermal stability of thermophilic l -threonine aldolase from Thermotoga maritima. Journal of Biotechnology, 2015, 199, 69-76. | 3.8 | 8 |
| 27 | Assessing Uncertainty in the Polish Agricultural Greenhouse Gas Emission Inventory Using Monte Carlo Simulation. Outlook on Agriculture, 2014, 43, 61-65. | 3.4 | 8 |
| 28 | BioShell-Threading: versatile Monte Carlo package for protein 3D threading. BMC Bioinformatics, 2014, 15, 22. | 2.6 | 17 |
| 29 | Coarse-Grained Protein Models in Structure Prediction. Springer Series in Bio-/neuroinformatics, 2014, , 25-53. | 0.1 | 1 |
| 30 | De Novo Protein Structure Determination from Incomplete Experimental Data. Biophysical Journal, 2013, 104, 228a. | 0.5 | 0 |
| 31 | Combining Coarse-Grained Protein Models with Replica-Exchange All-Atom Molecular Dynamics. International Journal of Molecular Sciences, 2013, 14, 9893-9905. | 4.1 | 22 |
| 32 | BioShell Threader: protein homology detection based on sequence profiles and secondary structure profiles. Nucleic Acids Research, 2012, 40, W257-W262. | 14.5 | 10 |
| 33 | 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 |
| 34 | Optimization of Profile-to-Profile Alignment Parameters for One-Dimensional Threading. Journal of Computational Biology, 2012, 19, 879-886. | 1.6 | 4 |
| 35 | 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. | 2.6 | 31 |
| 36 | Optimization of protein models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 479-493. | 14.6 | 32 |

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|---|---|---|---|
| 37 | Generalized Fragment Picking in Rosetta: Design, Protocols and Applications. PLoS ONE, 2011, 6, e23294. | 2.5 | 172 |
| 38 | The crystal structure of the AF2331 protein from <i>Archaeoglobus fulgidus</i> DSM 4304 forms an unusual interdigitated dimer with a new type of Î± + Î² fold. Protein Science, 2009, 18, 2410-2419. | 7.6 | 11 |
| 39 | Fast and accurate methods for predicting short-range constraints in protein models. Journal of Computer-Aided Molecular Design, 2008, 22, 783-788. | 2.9 | 0 |
| 40 | Utility library for structural bioinformatics. Bioinformatics, 2008, 24, 584-585. | 4.1 | 38 |
| 41 | Efficient scheme for optimization of parallel tempering Monte Carlo method. Journal of Physics Condensed Matter, 2007, 19, 036225. | 1.8 | 25 |
| 42 | Comparative modeling without implicit sequence alignments. Bioinformatics, 2007, 23, 2522-2527. | 4.1 | 16 |
| 43 | T-Pile a package for thermodynamic calculations for biomolecules. Bioinformatics, 2007, 23, 1840-1842. | 4.1 | 3 |
| 44 | 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. | 3.3 | 102 |
| 45 | 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 |
| 46 | Type II restriction endonuclease R.Eco29kI is a member of the GIY-YIG nuclease superfamily. BMC Structural Biology, 2007, 7, 48. | 2.3 | 32 |
| 47 | BioShell--a package of tools for structural biology computations. Bioinformatics, 2006, 22, 621-622. | 4.1 | 44 |
| 48 | Denatured proteins and early folding intermediates simulated in a reduced conformational space. Acta Biochimica Polonica, 2006, 53, 131-44. | 0.5 | 10 |
| 49 | Clustering as a supporting tool for structural drug design. Acta Poloniae Pharmaceutica, 2006, 63, 436-8. | 0.1 | 0 |
| 50 | Protein structure prediction by tempering spatial constraints. Journal of Computer-Aided Molecular Design, 2005, 19, 603-608. | 2.9 | 3 |
| 51 | Exploring protein energy landscapes with hierarchical clustering. International Journal of Quantum Chemistry, 2005, 105, 826-830. | 2.0 | 21 |
| 52 | HCPM--program for hierarchical clustering of protein models. Bioinformatics, 2005, 21, 3179-3180. | 4.1 | 30 |
| 53 | A new approach to prediction of short-range conformational propensities in proteins. Bioinformatics, 2005, 21, 981-987. | 4.1 | 8 |
| 54 | A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition. Biopolymers, 2003, 69, 399-405. | 2.4 | 21 |

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| 55 | A new combination of replica exchange Monte Carlo and histogram analysis for protein folding and thermodynamics. Journal of Chemical Physics, 2001, 115, 1569-1574. | 3.0 | 29 |
| 56 | 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. | 3.0 | 66 |