JiÅÃ- VondrÃ¡Å¡ek

List of Publications by Year
in descending order

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109	4,347	159585 30	118850 62
papers	citations	h-index	g-index

113	113	113	6301
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	TRPM5 Channel Binds Calcium-Binding Proteins Calmodulin and S100A1. Biochemistry, 2022, 61, 413-423.	2.5	1
2	Modern and prebiotic amino acids support distinct structural profiles in proteins. Open Biology, 2022, 12, .	3.6	11
3	Fusion of two unrelated protein domains in a chimera protein and its <scp>3D</scp> prediction: Justification of the xâ€ray reference structures as a prediction benchmark. Proteins: Structure, Function and Bioinformatics, 2022, 90, 2067-2079.	2.6	2
4	Intrinsically disordered protein domain of human ameloblastin in synthetic fusion with calmodulin increases calmodulin stability and modulates its function. International Journal of Biological Macromolecules, 2021, 168, 1-12.	7.5	3
5	ELIXIRâ€EXCELERATE: establishing Europe's data infrastructure for the life science research of the future. EMBO Journal, 2021, 40, e107409.	7.8	18
6	Enzyme catalysis prior to aromatic residues: Reverse engineering of a dephosphoâ€CoA kinase. Protein Science, 2021, 30, 1022-1034.	7.6	15
7	Amino Acid Interactions (INTAA) web server v2.0: a single service for computation of energetics and conservation in biomolecular 3D structures. Nucleic Acids Research, 2021, 49, W15-W20.	14.5	6
8	IDSM ChemWebRDF: SPARQLing small-molecule datasets. Journal of Cheminformatics, 2021, 13, 38.	6.1	10
9	The order of PDZ3 and TrpCage in fusion chimeras determines their propertiesâ€”a biophysical characterization. Protein Science, 2021, 30, 1653-1666.	7.6	1
10	TRPM7 N-terminal region forms complexes with calcium binding proteins CaM and S100A1. Heliyon, 2021, 7, e08490.	3.2	3
11	GigaSOM.jl: High-performance clustering and visualization of huge cytometry datasets. GigaScience, 2020, 9, .	6.4	8
12	Characterization of AMBN I and II Isoforms and Study of Their Ca2+-Binding Properties. International Journal of Molecular Sciences, 2020, 21, 9293.	4.1	9
13	Mapping of CaM, S100A1 and PIP2-Binding Epitopes in the Intracellular N- and C-Termini of TRPM4. International Journal of Molecular Sciences, 2020, 21, 4323.	4.1	6
14	Efficient Estimation of Absolute Binding Free Energy for a Homeodomainâ€“DNA Complex from Nonequilibrium Pulling Simulations. Journal of Chemical Theory and Computation, 2020, 16, 2034-2041.	5.3	7
15	Hydrophobic Amino Acids as Universal Elements of Protein-Induced DNA Structure Deformation. International Journal of Molecular Sciences, 2020, 21, 3986.	4.1	5
16	The bio.tools registry of software tools and data resources for the life sciences. Genome Biology, 2019, 20, 164.	8.8	39
17	Interoperable chemical structure search service. Journal of Cheminformatics, 2019, 11, 45.	6.1	12
18	TRPM6 N-Terminal CaM- and S100A1-Binding Domains. International Journal of Molecular Sciences, 2019, 20, 4430.	4.1	9

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19	Toward Ab Initio Protein Folding: Inherent Secondary Structure Propensity of Short Peptides from the Bioinformatics and Quantum-Chemical Perspective. Journal of Physical Chemistry B, 2019, 123, 1215-1227.	2.6	12
20	Can All-Atom Molecular Dynamics Simulations Quantitatively Describe Homeodomainâ€“DNA Binding Equilibria?. Journal of Chemical Theory and Computation, 2019, 15, 2635-2648.	5.3	8
21	Exquisite ligand stereoselectivity of a Drosophila juvenile hormone receptor contrasts with its broad agonist repertoire. Journal of Biological Chemistry, 2019, 294, 410-423.	3.4	37
22	AMBER and CHARMM Force Fields Inconsistently Portray the Microscopic Details of Phosphorylation. Journal of Chemical Theory and Computation, 2019, 15, 665-679.	5.3	18
23	Generalized EmbedSOM on quadtree-structured self-organizing maps. F1000Research, 2019, 8, 2120.	1.6	6
24	Generalized EmbedSOM on quadtree-structured self-organizing maps. F1000Research, 2019, 8, 2120.	1.6	6
25	Substituents at the C3â€² and C3â€²N positions are critical for taxanes to overcome acquired resistance of cancer cells to paclitaxel. Toxicology and Applied Pharmacology, 2018, 347, 79-91.	2.8	10
26	Novel Structural Mechanism of Allosteric Regulation of Aspartic Peptidases via an Evolutionarily Conserved Exosite. Cell Chemical Biology, 2018, 25, 318-329.e4.	5.2	14
27	Shared CaMâ€•and S100A1â€‰binding epitopes in the distal <scp>TRPM</scp>4 N terminus. FEBS Journal, 2018, 285, 599-613.	4.7	12
28	An ameloblastin C-terminus variant is present in human adipose tissue. Heliyon, 2018, 4, e01075.	3.2	3
29	Widespread evolutionary crosstalk among protein domains in the context of multi-domain proteins. PLoS ONE, 2018, 13, e0203085.	2.5	0
30	SmSP2: A serine protease secreted by the blood fluke pathogen Schistosoma mansoni with anti-hemostatic properties. PLoS Neglected Tropical Diseases, 2018, 12, e0006446.	3.0	26
31	Sachem: a chemical cartridge for high-performance substructure search. Journal of Cheminformatics, 2018, 10, 27.	6.1	18
32	Amino Acid Interaction (INTAA) web server. Nucleic Acids Research, 2017, 45, W388-W392.	14.5	38
33	Noncovalent Interactions in Specific Recognition Motifs of Proteinâ€“DNA Complexes. Journal of Chemical Theory and Computation, 2017, 13, 877-885.	5.3	22
34	Random protein sequences can form defined secondary structures and are well-tolerated in vivo. Scientific Reports, 2017, 7, 15449.	3.3	68
35	The identification of new substrates of human DHRS7 by molecular modeling and in vitro testing. International Journal of Biological Macromolecules, 2017, 105, 171-182.	7.5	4
36	Ameloblastin Peptides Modulates the Osteogenic Capacity of Human Mesenchymal Stem Cells. Frontiers in Physiology, 2017, 8, 58.	2.8	9

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37	Phosphorylation Modulates Ameloblastin Self-assembly and Ca2+ Binding. Frontiers in Physiology, 2017, 8, 531.	2.8	12
38	A community proposal to integrate proteomics activities in ELIXIR. F1000Research, 2017, 6, 875.	1.6	13
39	Regioselective Palmitoylation of 9-(2,3-Dihydroxy- propyl)adenine Catalyzed by a Glycopolymer-enzyme Conjugate. Molecules, 2016, 21, 648.	3.8	2
40	Artificial proteins as allosteric modulators of PDZ3 and SH3 in twoâ€domain constructs: A computational characterization of novel chimeric proteins. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1358-1374.	2.6	4
41	Advanced SPARQL querying in small molecule databases. Journal of Cheminformatics, 2016, 8, 31.	6.1	7
42	The characterization of a novel S100A1 binding site in the N-terminus of TRPM1. International Journal of Biochemistry and Cell Biology, 2016, 78, 186-193.	2.8	7
43	Insights into Unfolded Proteins from the Intrinsic Ï•/Ï^ Propensities of the AAXAA Host-Guest Series. Biophysical Journal, 2016, 110, 348-361.	0.5	12
44	Computational methods for the description of pharmacologically relevant platinum complexes â€“ molecular structure and bond dissociation. Physical Chemistry Chemical Physics, 2016, 18, 4051-4062.	2.8	4
45	Effect of TFE on the Helical Content of AK17 and HAL-1 Peptides: Theoretical Insights into the Mechanism of Helix Stabilization. Journal of Physical Chemistry B, 2016, 120, 1048-1059.	2.6	30
46	Sequence-Specific Recognition of DNA by Proteins: Binding Motifs Discovered Using a Novel Statistical/Computational Analysis. PLoS ONE, 2016, 11, e0158704.	2.5	10
47	Prolyl Oligopeptidase from the Blood Fluke Schistosoma mansoni: From Functional Analysis to Anti-schistosomal Inhibitors. PLoS Neglected Tropical Diseases, 2015, 9, e0003827.	3.0	34
48	PIP2 and PIP3 interact with N-terminus region of TRPM4 channel. Biophysical Chemistry, 2015, 205, 24-32.	2.8	25
49	Characterization of the part of N-terminal PIP2 binding site of the TRPM1 channel. Biophysical Chemistry, 2015, 207, 135-142.	2.8	9
50	Representative Amino Acid Side-Chain Interactions in Proteinâ€“DNA Complexes: A Comparison of Highly Accurate Correlated Ab Initio Quantum Mechanical Calculations and Efficient Approaches for Applications to Large Systems. Journal of Chemical Theory and Computation, 2015, 11, 4086-4092.	5.3	22
51	Large-Scale Quantitative Assessment of Binding Preferences in Proteinâ€“Nucleic Acid Complexes. Journal of Chemical Theory and Computation, 2015, 11, 1939-1948.	5.3	12
52	Trypsin- and Chymotrypsin-Like Serine Proteases in Schistosoma mansoni â€“ â€˜The Undiscovered Countryâ€™. PLoS Neglected Tropical Diseases, 2014, 8, e2766.	3.0	31
53	Activation Route of the Schistosoma mansoni Cathepsin B1 Drug Target: Structural Map with a Glycosaminoglycan Switch. Structure, 2014, 22, 1786-1798.	3.3	34
54	Retro operation on the Trp-cage miniprotein sequence produces an unstructured molecule capable of folding similar to the original only upon 2,2,2-trifluoroethanol addition. Protein Engineering, Design and Selection, 2014, 27, 463-472.	2.1	3

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55	Parametrization of 2,2,2-Trifluoroethanol Based on the Generalized Amber Force Field Provides Realistic Agreement between Experimental and Calculated Properties of Pure Liquid as Well as Water-Mixed Solutions. Journal of Physical Chemistry B, 2014, 118, 10390-10404.	2.6	22
56	On InChI and evaluating the quality of cross-reference links. Journal of Cheminformatics, 2014, 6, 15.	6.1	5
57	Highly selective purification of three lipases from Geotrichum candidum 4013 and their characterization and biotechnological applications. Journal of Molecular Catalysis B: Enzymatic, 2013, 98, 62-72.	1.8	26
58	Critical Assessment of Current Force Fields. Short Peptide Test Case. Journal of Chemical Theory and Computation, 2013, 9, 441-451.	5.3	29
59	Intrinsically Disordered Enamel Matrix Protein Ameloblastin Forms Ribbon-like Supramolecular Structures via an N-terminal Segment Encoded by Exon 5. Journal of Biological Chemistry, 2013, 288, 22333-22345.	3.4	36
60	Effect of Enamel Matrix Derivative and of Proline-Rich Synthetic Peptides on the Differentiation of Human Mesenchymal Stem Cells Toward the Osteogenic Lineage. Tissue Engineering - Part A, 2012, 18, 1253-1263.	3.1	27
61	Towards a better understanding of the specificity of proteinâ€“protein interaction. Journal of Molecular Recognition, 2012, 25, 604-615.	2.1	7
62	Optimal Definition of Inter-Residual Contact in Globular Proteins Based on Pairwise Interaction Energy Calculations, Its Robustness, and Applications. Journal of Physical Chemistry B, 2012, 116, 12651-12660.	2.6	5
63	Novel highâ€affinity binders of human interferon gamma derived from albuminâ€binding domain of protein G. Proteins: Structure, Function and Bioinformatics, 2012, 80, 774-789.	2.6	30
64	Urea and Guanidinium Induced Denaturation of a Trp-Cage Miniprotein. Journal of Physical Chemistry B, 2011, 115, 8910-8924.	2.6	56
65	Like-Charge Guanidinium Pairing from Molecular Dynamics and Ab Initio Calculations. Journal of Physical Chemistry A, 2011, 115, 11193-11201.	2.5	53
66	Mapping the Pro-Peptide of the Schistosoma mansoni Cathepsin B1 Drug Target: Modulation of Inhibition by Heparin and Design of Mimetic Inhibitors. ACS Chemical Biology, 2011, 6, 609-617.	3.4	34
67	Gyration- and Inertia-Tensor-Based Collective Coordinates for Metadynamics. Application on the Conformational Behavior of Polyalanine Peptides and Trp-Cage Folding. Journal of Physical Chemistry A, 2011, 115, 11455-11465.	2.5	48
68	Biophysical characterization of recombinant human ameloblastin. European Journal of Oral Sciences, 2011, 119, 261-269.	1.5	22
69	The DF-LCCSD(T0) correction of the Ï†/Ïˆ force field dihedral parameters significantly influences the free energy profile of the alanine dipeptide. Chemical Physics Letters, 2011, 503, 301-304.	2.6	10
70	How to fragment a polypeptide? An ab initio computational study of pair interactions between amino acids and ligand-amino acids in proteins. Collection of Czechoslovak Chemical Communications, 2011, 76, 605-618.	1.0	0
71	Hypertrophic cardiomyopathy: from mutation to functional analysis of defective protein. Croatian Medical Journal, 2011, 52, 384-391.	0.7	5
72	Synthetic Peptides Analogue to Enamel Proteins Promote Osteogenic Differentiation of MC3T3-E1 and Mesenchymal Stem Cells. Journal of Biomaterials and Tissue Engineering, 2011, 1, 198-209.	0.1	17

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73	Metadynamics As a Tool for Mapping the Conformational and Free-Energy Space of Peptides â€" The Alanine Dipeptide Case Study. Journal of Physical Chemistry B, 2010, 114, 5632-5642.	2.6	58
74	Energy Matrix of Structurally Important Side-Chain/Side-Chain Interactions in Proteins. Journal of Chemical Theory and Computation, 2010, 6, 2191-2203.	5.3	33
75	Analysis of Energy Stabilization inside the Hydrophobic Core of Rubredoxin. ChemPhysChem, 2009, 10, 543-548.	2.1	4
76	Loss of Dispersion Energy Changes the Stability and Folding/Unfolding Equilibrium of the Trp-Cage Protein. Journal of Physical Chemistry B, 2009, 113, 5657-5660.	2.6	21
77	Structure and Stability of the Waterâ"Graphite Complexes. Journal of Physical Chemistry C, 2009, 113, 8412-8419.	3.1	96
78	Ion specific effects of sodium and potassium on the catalytic activity of HIV-1 protease. Physical Chemistry Chemical Physics, 2009, 11, 7599.	2.8	36
79	Representative Amino Acid Side Chain Interactions in Proteins. A Comparison of Highly Accurate Correlatedab InitioQuantum Chemical and Empirical Potential Procedures. Journal of Chemical Theory and Computation, 2009, 5, 982-992.	5.3	89
80	Rigid Duplex Î±-Cyclodextrin Reversibly Connected With Disulfide Bonds. Synthesis and Inclusion Complexes. Journal of Organic Chemistry, 2009, 74, 1082-1092.	3.2	36
81	The Molecular Origin of Like-Charge Argineneâ"Arginine Pairing in Water. Journal of Physical Chemistry B, 2009, 113, 9041-9045.	2.6	142
82	Identifying stabilizing key residues in proteins using interresidue interaction energy matrix. Proteins: Structure, Function and Bioinformatics, 2008, 72, 402-413.	2.6	37
83	Another role of proline: stabilization interactions in proteins and protein complexes concerning proline and tryptophane. Physical Chemistry Chemical Physics, 2008, 10, 6350.	2.8	80
84	Bioinformatic analysis and molecular modelling of human ameloblastin suggest a twoâ€domain intrinsically unstructured calciumâ€binding protein. European Journal of Oral Sciences, 2008, 116, 124-134.	1.5	40
85	Quasiplanarity of the Peptide Bond. Journal of Physical Chemistry A, 2008, 112, 693-699.	2.5	15
86	MedusaScore: An Accurate Force Field-Based Scoring Function for Virtual Drug Screening. Journal of Chemical Information and Modeling, 2008, 48, 1656-1662.	5.4	165
87	Quantum Chemical Benchmark Energy and Geometry Database for Molecular Clusters and Complex Molecular Systems (www.begdb.com): A Users Manual and Examples. Collection of Czechoslovak Chemical Communications, 2008, 73, 1261-1270.	1.0	144
88	The Stabilization Energy of the GLU-LYS Salt Bridge in the Protein/Water Environment: Correlated Quantum Chemical ab initio, DFT and Empirical Potential Studies. Collection of Czechoslovak Chemical Communications, 2008, 73, 921-936.	1.0	2
89	Model of Peptide Bondâ"Aromatic Ring Interaction:Â Correlated Ab Initio Quantum Chemical Study. Journal of Physical Chemistry B, 2007, 111, 9975-9979.	2.6	34
90	Performance of the DFT-D method, paired with the PCM implicit solvation model, for the computation of interaction energies of solvated complexes of biological interest. Physical Chemistry Chemical Physics, 2007, 9, 5555.	2.8	63

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91	Dispersion Interactions Govern the Strong Thermal Stability of a Protein. Chemistry - A European Journal, 2007, 13, 9022-9027.	3.3	29
92	Thermodynamic Penalty Arising from Burial of a Ligand Polar Group Within a Hydrophobic Pocket of a Protein Receptor. Journal of Molecular Biology, 2006, 362, 994-1003.	4.2	39
93	Chemical compound navigator: A web-based chem-BLAST, chemical taxonomy-based search engine for browsing compounds. Proteins: Structure, Function and Bioinformatics, 2006, 63, 907-917.	2.6	13
94	Quantification and rationalization of the higher affinity of sodium over potassium to protein surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 15440-15444.	7.1	212
95	Application of InChI to curate, index, and query 3-D structures. Proteins: Structure, Function and Bioinformatics, 2005, 60, 1-4.	2.6	19
96	Homology modeling and SAR analysis of Schistosoma japonicum cathepsin D (SjCD) with statin inhibitors identify a unique active site steric barrier with potential for the design of specific inhibitors. Biological Chemistry, 2005, 386, 339-349.	2.5	16
97	Unexpectedly Strong Energy Stabilization Inside the Hydrophobic Core of Small Protein Rubredoxin Mediated by Aromatic Residues:Â Correlated Ab Initio Quantum Chemical Calculations. Journal of the American Chemical Society, 2005, 127, 2615-2619.	13.7	142
98	Sexual Attraction in the Silkworm Moth. Chemistry and Biology, 2003, 10, 331-340.	6.0	48
99	Unusual Binding Mode of an HIV-1 Protease Inhibitor Explains its Potency against Multi-drug-resistant Virus Strains. Journal of Molecular Biology, 2002, 324, 739-754.	4.2	46
100	Free-thiol Cys331 exposed during activation process is critical for native tetramer structure of cathepsin C (dipeptidyl peptidase I). Protein Science, 2002, 11, 933-943.	7.6	19
101	Magnesium and biological activity of oxytocin analogues modified on aromatic ring of amino acid in position 2. Journal of Peptide Science, 2001, 7, 413-424.	1.4	5
102	Solid phase synthesis of glycopeptide dendrimers with Tn antigenic structure and their biological activities. Part I. Journal of Peptide Science, 1999, 5, 46-55.	1.4	24
103	INHIBITORS OF HIV-1 PROTEASE: A Major Success of Structure-Assisted Drug Design. Annual Review of Biophysics and Biomolecular Structure, 1998, 27, 249-284.	18.3	649
104	Coordination geometries of selected transition metal ions (Co2+, Ni2+, Cu2+, Zn2+, Cd2+, and Hg2+) in metalloproteins. Journal of Inorganic Biochemistry, 1998, 71, 115-127.	3.5	363
105	Database of three-dimensional structures of HIV proteinases. Nature Structural and Molecular Biology, 1997, 4, 8-8.	8.2	51
106	Configurations of Diastereomeric Hydroxyethylene Isosteres Strongly Affect Biological Activities of a Series of Specific Inhibitors of Human-Immunodeficiency-Virus Proteinase. FEBS Journal, 1997, 250, 559-566.	0.2	25
107	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), andab initio Hartree-Fock method for interaction of DNA bases: Comparison with nonempirical beyond Hartree-Fock results. Journal of Computational Chemistry, 1997, 18, 1136-1150.	3.3	251
108	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), and ab initio Hartreeâ€“Fock method for interaction of DNA bases: Comparison with nonempirical beyond Hartreeâ€“Fock results. , 1997, 18, 1136.		2

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109	The LOTUS initiative for open knowledge management in natural products research. ELife, 0, 11, .	6.0	90