JiÅÃ- VondrÃ¡Å¡ek

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5299376/publications.pdf

Version: 2024-02-01

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	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
2	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
3	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
4	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
5	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
6	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
7	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
8	The Molecular Origin of Like-Charge Argineneâ^'Arginine Pairing in Water. Journal of Physical Chemistry B, 2009, 113, 9041-9045.	2.6	142
9	Structure and Stability of the Waterâ^'Graphite Complexes. Journal of Physical Chemistry C, 2009, 113, 8412-8419.	3.1	96
10	The LOTUS initiative for open knowledge management in natural products research. ELife, 0, 11, .	6.0	90
11	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
12	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
13	Random protein sequences can form defined secondary structures and are well-tolerated in vivo. Scientific Reports, 2017, 7, 15449.	3.3	68
14	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
15	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
16	Urea and Guanidinium Induced Denaturation of a Trp-Cage Miniprotein. Journal of Physical Chemistry B, 2011, 115, 8910-8924.	2.6	56
17	Like-Charge Guanidinium Pairing from Molecular Dynamics and Ab Initio Calculations. Journal of Physical Chemistry A, 2011, 115, 11193-11201.	2.5	53
18	Database of three-dimensional structures of HIV proteinases. Nature Structural and Molecular Biology, 1997, 4, 8-8.	8.2	51

#	ARTICLE	IF	CITATIONS
19	Sexual Attraction in the Silkworm Moth. Chemistry and Biology, 2003, 10, 331-340.	6.0	48
20	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
21	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
22	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
23	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
24	The bio.tools registry of software tools and data resources for the life sciences. Genome Biology, 2019, 20, 164.	8.8	39
25	Amino Acid Interaction (INTAA) web server. Nucleic Acids Research, 2017, 45, W388-W392.	14.5	38
26	Identifying stabilizing key residues in proteins using interresidue interaction energy matrix. Proteins: Structure, Function and Bioinformatics, 2008, 72, 402-413.	2.6	37
27	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
28	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
29	Rigid Duplex Î±-Cyclodextrin Reversibly Connected With Disulfide Bonds. Synthesis and Inclusion Complexes. Journal of Organic Chemistry, 2009, 74, 1082-1092.	3.2	36
30	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
31	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
32	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
33	Activation Route of the Schistosoma mansoni Cathepsin B1 Drug Target: Structural Map with a Glycosaminoglycan Switch. Structure, 2014, 22, 1786-1798.	3.3	34
34	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
35	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
36	Trypsin- and Chymotrypsin-Like Serine Proteases in Schistosoma mansoni â€“ â€˜The Undiscovered Countryâ€™. PLoS Neglected Tropical Diseases, 2014, 8, e2766.	3.0	31

#	ARTICLE	IF	CITATIONS
37	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
38	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
39	Dispersion Interactions Govern the Strong Thermal Stability of a Protein. Chemistry - A European Journal, 2007, 13, 9022-9027.	3.3	29
40	Critical Assessment of Current Force Fields. Short Peptide Test Case. Journal of Chemical Theory and Computation, 2013, 9, 441-451.	5.3	29
41	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
42	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
43	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
44	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
45	PIP2 and PIP3 interact with N-terminus region of TRPM4 channel. Biophysical Chemistry, 2015, 205, 24-32.	2.8	25
46	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
47	Biophysical characterization of recombinant human ameloblastin. European Journal of Oral Sciences, 2011, 119, 261-269.	1.5	22
48	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
49	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
50	Noncovalent Interactions in Specific Recognition Motifs of Proteinâ€“DNA Complexes. Journal of Chemical Theory and Computation, 2017, 13, 877-885.	5.3	22
51	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
52	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
53	Application of InChI to curate, index, and query 3-D structures. Proteins: Structure, Function and Bioinformatics, 2005, 60, 1-4.	2.6	19
54	Sachem: a chemical cartridge for high-performance substructure search. Journal of Cheminformatics, 2018, 10, 27.	6.1	18

#	Article	IF	Citations
55	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
56	ELIXIRâ€ŁXCELERATE: establishing Europe's data infrastructure for the life science research of the future. EMBO Journal, 2021, 40, e107409.	7.8	18
57	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
58	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
59	Quasiplanarity of the Peptide Bond. Journal of Physical Chemistry A, 2008, 112, 693-699.	2.5	15
60	Enzyme catalysis prior to aromatic residues: Reverse engineering of a dephosphoâ€ŁCoA kinase. Protein Science, 2021, 30, 1022-1034.	7.6	15
61	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
62	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
63	A community proposal to integrate proteomics activities in ELIXIR. F1000Research, 2017, 6, 875.	1.6	13
64	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
65	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
66	Phosphorylation Modulates Ameloblastin Self-assembly and Ca2+ Binding. Frontiers in Physiology, 2017, 8, 531.	2.8	12
67	Shared CaMâ€•and S100A1â€binding epitopes in the distal <scp>TRPM</scp>4 N terminus. FEBS Journal, 2018, 285, 599-613.	4.7	12
68	Interoperable chemical structure search service. Journal of Cheminformatics, 2019, 11, 45.	6.1	12
69	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
70	Modern and prebiotic amino acids support distinct structural profiles in proteins. Open Biology, 2022, 12, .	3.6	11
71	The DF-LCCSD(T0) correction of the Ï†/Ï^ force field dihedral parameters significantly influences the free energy profile of the alanine dipeptide. Chemical Physics Letters, 2011, 503, 301-304.	2.6	10
72	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

#	Article	IF	Citations
73	IDSM ChemWebRDF: SPARQLing small-molecule datasets. Journal of Cheminformatics, 2021, 13, 38.	6.1	10
74	Sequence-Specific Recognition of DNA by Proteins: Binding Motifs Discovered Using a Novel Statistical/Computational Analysis. PLoS ONE, 2016, 11, e0158704.	2.5	10
75	Characterization of the part of N-terminal PIP2 binding site of the TRPM1 channel. Biophysical Chemistry, 2015, 207, 135-142.	2.8	9
76	Ameloblastin Peptides Modulates the Osteogenic Capacity of Human Mesenchymal Stem Cells. Frontiers in Physiology, 2017, 8, 58.	2.8	9
77	TRPM6 N-Terminal CaM- and S100A1-Binding Domains. International Journal of Molecular Sciences, 2019, 20, 4430.	4.1	9
78	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
79	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
80	GigaSOM.jl: High-performance clustering and visualization of huge cytometry datasets. GigaScience, 2020, 9, .	6.4	8
81	Towards a better understanding of the specificity of proteinâ€“protein interaction. Journal of Molecular Recognition, 2012, 25, 604-615.	2.1	7
82	Advanced SPARQL querying in small molecule databases. Journal of Cheminformatics, 2016, 8, 31.	6.1	7
83	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
84	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
85	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
86	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
87	Generalized EmbedSOM on quadtree-structured self-organizing maps. F1000Research, 2019, 8, 2120.	1.6	6
88	Generalized EmbedSOM on quadtree-structured self-organizing maps. F1000Research, 2019, 8, 2120.	1.6	6
89	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
90	Hypertrophic cardiomyopathy: from mutation to functional analysis of defective protein. Croatian Medical Journal, 2011, 52, 384-391.	0.7	5

#	Article	IF	Citations
91	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
92	On InChI and evaluating the quality of cross-reference links. Journal of Cheminformatics, 2014, 6, 15.	6.1	5
93	Hydrophobic Amino Acids as Universal Elements of Protein-Induced DNA Structure Deformation. International Journal of Molecular Sciences, 2020, 21, 3986.	4.1	5
94	Analysis of Energy Stabilization inside the Hydrophobic Core of Rubredoxin. ChemPhysChem, 2009, 10, 543-548.	2.1	4
95	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
96	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
97	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
98	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
99	An ameloblastin C-terminus variant is present in human adipose tissue. Heliyon, 2018, 4, e01075.	3.2	3
100	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
101	TRPM7 N-terminal region forms complexes with calcium binding proteins CaM and S100A1. Heliyon, 2021, 7, e08490.	3.2	3
102	Regioselective Palmitoylation of 9-(2,3-Dihydroxy- propyl)adenine Catalyzed by a Glycopolymer-enzyme Conjugate. Molecules, 2016, 21, 648.	3.8	2
103	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
104	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
105	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
106	The order of PDZ3 and TrpCage in fusion chimeras determines their propertiesâ€”a biophysical characterization. Protein Science, 2021, 30, 1653-1666.	7.6	1
107	TRPM5 Channel Binds Calcium-Binding Proteins Calmodulin and S100A1. Biochemistry, 2022, 61, 413-423.	2.5	1
108	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

#	ARTICLE	IF	CITATIONS
109	Widespread evolutionary crosstalk among protein domains in the context of multi-domain proteins. PLoS ONE, 2018, 13, e0203085.	2.5	0