Istvan Simon

List of Publications by Year in descending order

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133 papers	12,504 citations	38742 50 h-index	24982 109 g-index
137 all docs	137 docs citations	137 times ranked	14222 citing authors

#	Article	IF	Citations
1	IUPred: web server for the prediction of intrinsically unstructured regions of proteins based on estimated energy content. Bioinformatics, 2005, 21, 3433-3434.	4.1	1,832
2	Principles governing amino acid composition of integral membrane proteins: application to topology prediction 1 1Edited by J. Thornton. Journal of Molecular Biology, 1998, 283, 489-506.	4.2	1,023
3	The Pairwise Energy Content Estimated from Amino Acid Composition Discriminates between Folded and Intrinsically Unstructured Proteins. Journal of Molecular Biology, 2005, 347, 827-839.	4.2	911
4	ANCHOR: web server for predicting protein binding regions in disordered proteins. Bioinformatics, 2009, 25, 2745-2746.	4.1	527
5	Prediction of Protein Binding Regions in Disordered Proteins. PLoS Computational Biology, 2009, 5, e1000376.	3.2	523
6	Preformed Structural Elements Feature in Partner Recognition by Intrinsically Unstructured Proteins. Journal of Molecular Biology, 2004, 338, 1015-1026.	4.2	494
7	PSORT-B: improving protein subcellular localization prediction for Gram-negative bacteria. Nucleic Acids Research, 2003, 31, 3613-3617.	14.5	383
8	Local structural disorder imparts plasticity on linear motifs. Bioinformatics, 2007, 23, 950-956.	4.1	376
9	Hydrogen exchange and the dynamic structure of proteins. Molecular and Cellular Biochemistry, 1982, 48, 135-160.	3.1	341
10	Disorder and Sequence Repeats in Hub Proteins and Their Implications for Network Evolution. Journal of Proteome Research, 2006, 5, 2985-2995.	3.7	312
11	PDB_TM: selection and membrane localization of transmembrane proteins in the protein data bank. Nucleic Acids Research, 2004, 33, D275-D278.	14.5	245
12	PDBTM: Protein Data Bank of transmembrane proteins after 8 years. Nucleic Acids Research, 2012, 41, D524-D529.	14.5	245
13	Molecular Principles of the Interactions of Disordered Proteins. Journal of Molecular Biology, 2007, 372, 549-561.	4.2	242
14	Close encounters of the third kind: disordered domains and the interactions of proteins. BioEssays, 2009, 31, 328-335.	2.5	229
15	Transmembrane proteins in the Protein Data Bank: identification and classification. Bioinformatics, 2004, 20, 2964-2972.	4.1	216
16	Malleable machines take shape in eukaryotic transcriptional regulation. Nature Chemical Biology, 2008, 4, 728-737.	8.0	192
17	BiSearch: primer-design and search tool for PCR on bisulfite-treated genomes. Nucleic Acids Research, 2005, 33, e9-e9.	14.5	159
18	Stabilization centers in proteins:Identification, characterization and predictions. Journal of Molecular Biology, 1997, 272, 597-612.	4.2	144

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19	Dynamic proteinâ€“DNA recognition: beyond what can be seen. Trends in Biochemical Sciences, 2011, 36, 415-423.	7.5	137
20	TMDET: web server for detecting transmembrane regions of proteins by using their 3D coordinates. Bioinformatics, 2005, 21, 1276-1277.	4.1	132
21	On filtering false positive transmembrane protein predictions. Protein Engineering, Design and Selection, 2002, 15, 745-752.	2.1	128
22	The role of hydrophobic microenvironments in modulating pKa shifts in proteins. Proteins: Structure, Function and Bioinformatics, 2002, 48, 283-292.	2.6	128
23	Rod models of DNA: sequence-dependent anisotropic elastic modelling of local bending phenomena. Trends in Biochemical Sciences, 1998, 23, 341-347.	7.5	122
24	Prevalent Structural Disorder inE.coliandS.cerevisiaeProteomes. Journal of Proteome Research, 2006, 5, 1996-2000.	3.7	119
25	TM or not TM: transmembrane protein prediction with low false positive rate using DAS-TMfilter. Bioinformatics, 2004, 20, 136-137.	4.1	113
26	Malleable Machines in Transcription Regulation: The Mediator Complex. PLoS Computational Biology, 2008, 4, e1000243.	3.2	109
27	SRide: a server for identifying stabilizing residues in proteins. Nucleic Acids Research, 2005, 33, W303-W305.	14.5	107
28	Bioinformatical approaches to characterize intrinsically disordered/unstructured proteins. Briefings in Bioinformatics, 2010, 11, 225-243.	6.5	107
29	SCide: identification of stabilization centers in proteins. Bioinformatics, 2003, 19, 899-900.	4.1	99
30	The BiSearch web server. BMC Bioinformatics, 2006, 7, 431.	2.6	86
31	Chaos game representation of protein structures. Journal of Molecular Graphics, 1994, 12, 302-304.	1.1	81
32	QM/MM simulation of liquid water with an adaptive quantum region. Physical Chemistry Chemical Physics, 2012, 14, 646-656.	2.8	80
33	Locating the stabilizing residues in (Î±/Î²)8 barrel proteins based on hydrophobicity, long-range interactions, and sequence conservation. Proteins: Structure, Function and Bioinformatics, 2004, 55, 316-329.	2.6	73
34	TOPDB: topology data bank of transmembrane proteins. Nucleic Acids Research, 2007, 36, D234-D239.	14.5	73
35	DIBS: a repository of disordered binding sites mediating interactions with ordered proteins. Bioinformatics, 2018, 34, 535-537.	4.1	72
36	Prediction of Protein Disorder at the Domain Level. Current Protein and Peptide Science, 2007, 8, 161-171.	1.4	71

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37	Membrane topology of human ABC proteins. FEBS Letters, 2006, 580, 1017-1022.	2.8	70
38	The effect of iron binding on the conformation of transferrin. A small angle x-ray scattering study. Biophysical Journal, 1985, 48, 799-802.	0.5	66
39	Role of Base Flipping in Specific Recognition of Damaged DNA by Repair Enzymes. Journal of Molecular Biology, 2002, 323, 823-834.	4.2	64
40	Conformation of human IgG subclasses in solution. Small-angle X-ray scattering and hydrodynamic studies. FEBS Journal, 1985, 147, 17-25.	0.2	63
41	Disordered Tails of Homeodomains Facilitate DNA Recognition by Providing a Trade-Off between Folding and Specific Binding. Journal of the American Chemical Society, 2009, 131, 15084-15085.	13.7	61
42	MFIB: a repository of protein complexes with mutual folding induced by binding. Bioinformatics, 2017, 33, 3682-3684.	4.1	61
43	Disordered Binding Regions and Linear Motifsâ€"Bridging the Gap between Two Models of Molecular Recognition. PLoS ONE, 2012, 7, e46829.	2.5	60
44	Different sequence environments of cysteines and half cystines in proteins Application to predict disulfide forming residues. FEBS Letters, 1992, 302, 117-120.	2.8	58
45	The expanding view of proteinâ€"protein interactions: complexes involving intrinsically disordered proteins. Physical Biology, 2011, 8, 035003.	1.8	55
46	New Alignment Strategy for Transmembrane Proteins. Journal of Molecular Biology, 1994, 243, 388-396.	4.2	54
47	Evaluating Boundary Dependent Errors in QM/MM Simulations. Journal of Physical Chemistry B, 2009, 113, 5728-5735.	2.6	53
48	Calculation of protein conformation as an assembly of stable overlapping segments: application to bovine pancreatic trypsin inhibitor.. Proceedings of the National Academy of Sciences of the United States of America, 1991, 88, 3661-3665.	7.1	52
49	Structure of cellulose. 2. Low-energy crystalline arrangements. Macromolecules, 1988, 21, 990-998.	4.8	51
50	The Role of Dimerization in Prion Replication. Biophysical Journal, 2002, 82, 1711-1718.	0.5	51
51	Flexibility of prolyl oligopeptidase: Molecular dynamics and molecular framework analysis of the potential substrate pathways. Proteins: Structure, Function and Bioinformatics, 2005, 60, 504-512.	2.6	51
52	Interfacial Water as a â€œHydration Fingerprintâ€• in the Noncognate Complex of BamHI. Biophysical Journal, 2005, 89, 903-911.	0.5	49
53	Conformational Energy Calculations of the Effects of Sequence Variations on the Conformations of Two Tetrapeptides. Macromolecules, 1978, 11, 797-804.	4.8	48
54	Is there a biological cost of protein disorder? Analysis of cancer-associated mutations. Molecular BioSystems, 2012, 8, 296-307.	2.9	43

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55	Flexible segments modulate co-folding of dUTPase and nucleocapsid proteins. Nucleic Acids Research, 2006, 35, 495-505.	14.5	42
56	A possible way for prediction of domain boundaries in globular proteins from amino acid sequence. Biochemical and Biophysical Research Communications, 1986, 139, 11-17.	2.1	40
57	Structure of cellulose. 1. Low-energy conformations of single chains. Macromolecules, 1988, 21, 983-990.	4.8	38
58	Topology of Membrane Proteins. Journal of Chemical Information and Computer Sciences, 2001, 41, 364-368.	2.8	37
59	Impact of Ligand Protonation on Virtual Screening against Î²-Secretase (BACE1). Journal of Chemical Information and Modeling, 2007, 47, 2366-2373.	5.4	37
60	The Energy Gap as a Universal Reaction Coordinate for the Simulation of Chemical Reactions. Journal of Physical Chemistry B, 2009, 113, 7867-7873.	2.6	36
61	Substrate Preference of Transglutaminase 2 Revealed by Logistic Regression Analysis and Intrinsic Disorder Examination. Journal of Molecular Biology, 2008, 383, 390-402.	4.2	35
62	Prion protein: Evolution caught en route. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 4431-4436.	7.1	34
63	Characteristic sequential residue environment of amino acids in proteins. International Journal of Peptide and Protein Research, 1986, 27, 483-492.	0.1	34
64	Topology Prediction of Helical Transmembrane Proteins: How Far Have We Reached?. Current Protein and Peptide Science, 2010, 11, 550-561.	1.4	32
65	Phosphorylation-induced transient intrinsic structure in the kinase-inducible domain of CREB facilitates its recognition by the KIX domain of CBP. Proteins: Structure, Function and Bioinformatics, 2006, 64, 749-757.	2.6	31
66	Predicting isomorphic residue replacements for protein design. International Journal of Peptide and Protein Research, 1990, 36, 236-239.	0.1	31
67	Regularities in the primary structure of proteins. International Journal of Peptide and Protein Research, 2009, 34, 184-195.	0.1	30
68	Nucleotide pyrophosphatase employs a P-loop-like motif to enhance catalytic power and NDP/NTP discrimination. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 14437-14442.	7.1	30
69	Study of the Position of NAD and Its Effect on the Conformation of d-Glyceraldehyde-3-phosphate Dehydrogenase by Small-Angle X-Ray Scattering. FEBS Journal, 1972, 30, 184-189.	0.2	28
70	Studies on the active center of pancreatic amylase. Molecular and Cellular Biochemistry, 1974, 4, 205-209.	3.1	28
71	TOPDOM: database of domains and motifs with conservative location in transmembrane proteins. Bioinformatics, 2008, 24, 1469-1470.	4.1	28
72	Probing the Two-Metal Ion Mechanism in the Restriction Endonuclease BamHI. Biochemistry, 2007, 46, 14514-14523.	2.5	27

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73	EPIC-DB: a proteomics database for studying Apicomplexan organisms. BMC Genomics, 2009, 10, 38.	2.8	26
74	CMWeb: an interactive on-line tool for analysing residue-residue contacts and contact prediction methods. Nucleic Acids Research, 2012, 40, W329-W333.	14.5	26
75	Conservation of amino acids in multiple alignments: aspartic acid has unexpected conservation. FEBS Letters, 1996, 397, 225-229.	2.8	24
76	A repetitive sequence of Epsteinâ€“Barr virus nuclear antigen 6 comprises overlapping T cell epitopes which induce HLA-DR-restricted CD4+ T lymphocytes. International Immunology, 2000, 12, 281-293.	4.0	24
77	Function-Related Regulation of the Stability of MHC Proteins. Biophysical Journal, 2000, 79, 2305-2313.	0.5	23
78	Electrostatic versus Nonelectrostatic Effects in DNA Sequence Discrimination by Divalent Ions Mg2+and Mn2+. Journal of Physical Chemistry B, 2007, 111, 6272-6279.	2.6	23
79	Computation of low-energy crystalline arrangements of cellulose triacetate. Macromolecules, 1992, 25, 709-720.	4.8	22
80	Combination of 2D/3D Ligand-Based Similarity Search in Rapid Virtual Screening from Multimillion Compound Repositories. Selection and Biological Evaluation of Potential PDE4 and PDE5 Inhibitors. Molecules, 2014, 19, 7008-7039.	3.8	22
81	Proteins with Complex Architecture as Potential Targets for Drug Design: A Case Study of Mycobacterium tuberculosis. PLoS Computational Biology, 2011, 7, e1002118.	3.2	21
82	Towards Proteomic Approaches for the Identification of Structural Disorder. Current Protein and Peptide Science, 2007, 8, 173-179.	1.4	20
83	The role of DNA bending in Cro protein-DNA interactions. Biophysical Chemistry, 1997, 69, 153-160.	2.8	19
84	â€˜Rapid evolutionâ€™ of the amino acid composition of proteins. Trends in Biochemical Sciences, 1990, 15, 135-136.	7.5	18
85	Molecular dynamics approach to study the discrepancies in the thermal behavior of amylose and chitosan conformations. Computational and Theoretical Chemistry, 2006, 764, 133-140.	1.5	18
86	Different segmental flexibility of human serum transferrin and lactoferrin. Archives of Biochemistry and Biophysics, 1989, 275, 181-184.	3.0	17
87	Protein stability indicates divergent evolution of PD-(D/E)XK type II restriction endonucleases. Protein Science, 2002, 11, 1978-1983.	7.6	17
88	Studies on the active center of pancreatic amylase. Molecular and Cellular Biochemistry, 1974, 4, 211-216.	3.1	16
89	Different sequence environments of amino acid residues involved and not involved in longâ€range interactions in proteins. International Journal of Peptide and Protein Research, 1994, 43, 205-208.	0.1	16
90	Predicting protein conformation by statistical methods. BBA - Proteins and Proteomics, 2001, 1549, 123-136.	2.1	15

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91	Systematic analysis of somatic mutations driving cancer: uncovering functional protein regions in disease development. Biology Direct, 2016, 11, 23.	4.6	15
92	Assessing Conservation of Disordered Regions in Proteins. The Open Proteomics Journal, 2008, 1, 46-53.	0.4	15
93	Effect of trypsin binding on the hydrogen exchange kinetics of bovine pancreatic trypsin inhibitor .beta.-sheet NH's. Biochemistry, 1984, 23, 2064-2068.	2.5	14
94	Mapping of a Protective Helper T Cell Epitope of Human Influenza A Virus Hemagglutinin. Biochemical and Biophysical Research Communications, 2000, 270, 190-198.	2.1	14
95	Role of stabilization centers in 4 helix bundle proteins. Proteins: Structure, Function and Bioinformatics, 2002, 48, 320-326.	2.6	14
96	Investigation of protein refolding: a special feature of native structure responsible for refolding ability. Journal of Theoretical Biology, 1985, 113, 703-710.	1.7	13
97	Predicting Redox State of Cysteines in Proteins. Methods in Enzymology, 2002, 353, 10-21.	1.0	13
98	Identification of potential glutaminyl cyclase inhibitors from lead-like libraries by in silico and in vitro fragment-based screening. Molecular Diversity, 2017, 21, 175-186.	3.9	13
99	Determination of small alterations in the radius of gyration by small-angle X-ray scattering. Journal of Applied Crystallography, 1971, 4, 317-318.	4.5	12
100	Stabilization centers and protein stability. Theoretical Chemistry Accounts, 2001, 106, 121-127.	1.4	12
101	Servers for sequence-structure relationship analysis and prediction. Nucleic Acids Research, 2003, 31, 3359-3363.	14.5	12
102	Sequential, Structural and FunctionalÂProperties of Protein Complexes Are Defined by How Folding and Binding Intertwine. Journal of Molecular Biology, 2019, 431, 4408-4428.	4.2	12
103	Metal-binding sites at the active site of restriction endonuclease BamHI can conform to a one-ion mechanism. Biological Chemistry, 2007, 388, 73-8.	2.5	10
104	The role of stabilization centers in protein thermal stability. Biochemical and Biophysical Research Communications, 2016, 471, 57-62.	2.1	9
105	Prediction and Analysis of Intrinsically Disordered Proteins. Methods in Molecular Biology, 2015, 1261, 35-59.	0.9	9
106	Stabilization centers in various proteins. Theoretical Chemistry Accounts, 1999, 101, 27-32.	1.4	8
107	Functionally and structurally relevant residues of enzymes: are they segregated or overlapping?. FEBS Letters, 2004, 567, 239-242.	2.8	8
108	Modeling MHC class II molecules and their bound peptides as expressed at the cell surface. Molecular Immunology, 2002, 38, 681-687.	2.2	7

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109	Noncovalent Cross-links in Context with Other Structural and Functional Elements of Proteinsâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 347-351.	2.8	7
110	Analysis of Heterodimeric â€œMutual Synergistic Foldingâ€•Complexes. International Journal of Molecular Sciences, 2019, 20, 5136.	4.1	7
111	The role of long-range interactions in defining the secondary structure of proteins is overestimated. Bioinformatics, 1997, 13, 297-301.	4.1	6
112	Active site residue involvement in monoamine or diamine oxidation catalysed by pea seedling amine oxidase. FEBS Journal, 2011, 278, 1232-1243.	4.7	6
113	Combination of Pharmacophore Matching, 2D Similarity Search, and In Vitro Biological Assays in the Selection of Potential 5â€HT₆ Antagonists from Large Commercial Repositories. Chemical Biology and Drug Design, 2015, 86, 864-880.	3.2	6
114	Physical Background of the Disordered Nature of â€œMutual Synergetic Foldingâ€•Proteins. International Journal of Molecular Sciences, 2018, 19, 3340.	4.1	6
115	Investigation of protein folding: Uneven distribution of point mutations along polypeptide chains. Journal of Theoretical Biology, 1979, 81, 247-258.	1.7	5
116	Proteins as general crystals. Journal of Theoretical Biology, 1986, 123, 121-124.	1.7	5
117	Independence divergence-generated binary trees of amino acids. Protein Engineering, Design and Selection, 1995, 8, 417-423.	2.1	5
118	Self-regulating genes. Exact steady state solution by using Poisson representation. Open Physics, 2014, 12, .	1.7	5
119	Series of Concentration-Induced Phase Transitions in Cholesterol/Phosphatidylcholine Mixtures. Biophysical Journal, 2013, 104, 2448-2455.	0.5	4
120	Subunit contact surfaceâ€”an additional argument in favour of continuous folding during biosynthesis of proteins. Journal of Theoretical Biology, 1980, 82, 685-688.	1.7	3
121	An EcoRIâ€“RsrI chimeric restriction endonuclease retains parental sequence specificity. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2007, 1774, 583-594.	2.3	3
122	Sequence and Structure Properties Uncover the Natural Classification of Protein Complexes Formed by Intrinsically Disordered Proteins via Mutual Synergistic Folding. International Journal of Molecular Sciences, 2019, 20, 5460.	4.1	3
123	Possible mechanism for the dynamic stabilization of protein structure. Journal of Theoretical Biology, 1981, 90, 487-493.	1.7	2
124	Electrostatic effect of trypsin binding on the hydrogen exchange rate of bovine pancreatic trypsin inhibitor Î²-sheet NH's. Journal of Theoretical Biology, 1985, 117, 505-508.	1.7	2
125	Proteins as special subsets of polypeptides. Journal of Biosciences, 1995, 20, 579-590.	1.1	2
126	A word of caution about biological inference â€“ Revisiting cysteine covalent state predictions. FEBS Open Bio, 2014, 4, 310-314.	2.3	2

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127	Macromolecular Interactions of Disordered Proteins. International Journal of Molecular Sciences, 2020, 21, 504.	4.1	2
128	Origin of Increased Solvent Accessibility of Peptide Bonds in Mutual Synergetic Folding Proteins. International Journal of Molecular Sciences, 2021, 22, 13404.	4.1	2
129	Bioinformatical Approaches to Unstructured/Disordered Proteins and Their Interactions. Springer Series in Bio-/neuroinformatics, 2014, , 525-556.	0.1	1
130	Repetitive elements of protein sequences as fossils of early life. Journal of Biological Physics, 1995, 20, 331-334.	1.5	0
131	Bioinformatical Approaches to Unstructured/Disordered Proteins and Their Complexes. Springer Series on Bio- and Neurosystems, 2019, , 561-596.	0.2	0
132	Resource for structure related information on transmembrane proteins. , 2010, , 45-59.		0
133	Assortment of Frontiers in Protein Science. International Journal of Molecular Sciences, 2022, 23, 3685.	4.1	0