Istvan Simon

List of Publications by Year in descending order

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133 papers	12,504 citations	44444 50 h-index	28425 109 g-index
137 all docs	137 docs citations	137 times ranked	15991 citing authors

#	Article	IF	Citations
1	Assortment of Frontiers in Protein Science. International Journal of Molecular Sciences, 2022, 23, 3685.	1.8	0
2	Origin of Increased Solvent Accessibility of Peptide Bonds in Mutual Synergetic Folding Proteins. International Journal of Molecular Sciences, 2021, 22, 13404.	1.8	2
3	Macromolecular Interactions of Disordered Proteins. International Journal of Molecular Sciences, 2020, 21, 504.	1.8	2
4	Analysis of Heterodimeric â€œMutual Synergistic Foldingâ€•Complexes. International Journal of Molecular Sciences, 2019, 20, 5136.	1.8	7
5	Sequential, Structural and FunctionalÂProperties of Protein Complexes Are Defined by How Folding and Binding Intertwine. Journal of Molecular Biology, 2019, 431, 4408-4428.	2.0	12
6	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.	1.8	3
7	Bioinformatical Approaches to Unstructured/Disordered Proteins and Their Complexes. Springer Series on Bio- and Neurosystems, 2019, , 561-596.	0.2	0
8	DIBS: a repository of disordered binding sites mediating interactions with ordered proteins. Bioinformatics, 2018, 34, 535-537.	1.8	72
9	Physical Background of the Disordered Nature of â€œMutual Synergetic Foldingâ€•Proteins. International Journal of Molecular Sciences, 2018, 19, 3340.	1.8	6
10	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.	2.1	13
11	MFIB: a repository of protein complexes with mutual folding induced by binding. Bioinformatics, 2017, 33, 3682-3684.	1.8	61
12	Systematic analysis of somatic mutations driving cancer: uncovering functional protein regions in disease development. Biology Direct, 2016, 11, 23.	1.9	15
13	The role of stabilization centers in protein thermal stability. Biochemical and Biophysical Research Communications, 2016, 471, 57-62.	1.0	9
14	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.	1.5	6
15	Prediction and Analysis of Intrinsically Disordered Proteins. Methods in Molecular Biology, 2015, 1261, 35-59.	0.4	9
16	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.	1.7	22
17	A word of caution about biological inference â€“ Revisiting cysteine covalent state predictions. FEBS Open Bio, 2014, 4, 310-314.	1.0	2
18	Bioinformatical Approaches to Unstructured/Disordered Proteins and Their Interactions. Springer Series in Bio-/neuroinformatics, 2014, , 525-556.	0.1	1

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19	Self-regulating genes. Exact steady state solution by using Poisson representation. Open Physics, 2014, 12, .	0.8	5
20	Series of Concentration-Induced Phase Transitions in Cholesterol/Phosphatidylcholine Mixtures. Biophysical Journal, 2013, 104, 2448-2455.	0.2	4
21	CMWeb: an interactive on-line tool for analysing residue-residue contacts and contact prediction methods. Nucleic Acids Research, 2012, 40, W329-W333.	6.5	26
22	PDBTM: Protein Data Bank of transmembrane proteins after 8 years. Nucleic Acids Research, 2012, 41, D524-D529.	6.5	245
23	QM/MM simulation of liquid water with an adaptive quantum region. Physical Chemistry Chemical Physics, 2012, 14, 646-656.	1.3	80
24	Is there a biological cost of protein disorder? Analysis of cancer-associated mutations. Molecular BioSystems, 2012, 8, 296-307.	2.9	43
25	Disordered Binding Regions and Linear Motifsâ€"Bridging the Gap between Two Models of Molecular Recognition. PLoS ONE, 2012, 7, e46829.	1.1	60
26	The expanding view of proteinâ€"protein interactions: complexes involving intrinsically disordered proteins. Physical Biology, 2011, 8, 035003.	0.8	55
27	Active site residue involvement in monoamine or diamine oxidation catalysed by pea seedling amine oxidase. FEBS Journal, 2011, 278, 1232-1243.	2.2	6
28	Dynamic proteinâ€"DNA recognition: beyond what can be seen. Trends in Biochemical Sciences, 2011, 36, 415-423.	3.7	137
29	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.	3.3	30
30	Proteins with Complex Architecture as Potential Targets for Drug Design: A Case Study of Mycobacterium tuberculosis. PLoS Computational Biology, 2011, 7, e1002118.	1.5	21
31	Topology Prediction of Helical Transmembrane Proteins: How Far Have We Reached?. Current Protein and Peptide Science, 2010, 11, 550-561.	0.7	32
32	Bioinformatical approaches to characterize intrinsically disordered/unstructured proteins. Briefings in Bioinformatics, 2010, 11, 225-243.	3.2	107
33	Resource for structure related information on transmembrane proteins. , 2010, , 45-59.		0
34	ANCHOR: web server for predicting protein binding regions in disordered proteins. Bioinformatics, 2009, 25, 2745-2746.	1.8	527
35	Prediction of Protein Binding Regions in Disordered Proteins. PLoS Computational Biology, 2009, 5, e1000376.	1.5	523
36	EPIC-DB: a proteomics database for studying Apicomplexan organisms. BMC Genomics, 2009, 10, 38.	1.2	26

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37	Regularities in the primary structure of proteins. International Journal of Peptide and Protein Research, 2009, 34, 184-195.	0.1	30
38	Close encounters of the third kind: disordered domains and the interactions of proteins. BioEssays, 2009, 31, 328-335.	1.2	229
39	Evaluating Boundary Dependent Errors in QM/MM Simulations. Journal of Physical Chemistry B, 2009, 113, 5728-5735.	1.2	53
40	The Energy Gap as a Universal Reaction Coordinate for the Simulation of Chemical Reactions. Journal of Physical Chemistry B, 2009, 113, 7867-7873.	1.2	36
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.	6.6	61
42	Malleable machines take shape in eukaryotic transcriptional regulation. Nature Chemical Biology, 2008, 4, 728-737.	3.9	192
43	Substrate Preference of Transglutaminase 2 Revealed by Logistic Regression Analysis and Intrinsic Disorder Examination. Journal of Molecular Biology, 2008, 383, 390-402.	2.0	35
44	Malleable Machines in Transcription Regulation: The Mediator Complex. PLoS Computational Biology, 2008, 4, e1000243.	1.5	109
45	TOPDOM: database of domains and motifs with conservative location in transmembrane proteins. Bioinformatics, 2008, 24, 1469-1470.	1.8	28
46	Assessing Conservation of Disordered Regions in Proteins. The Open Proteomics Journal, 2008, 1, 46-53.	0.4	15
47	Prediction of Protein Disorder at the Domain Level. Current Protein and Peptide Science, 2007, 8, 161-171.	0.7	71
48	Towards Proteomic Approaches for the Identification of Structural Disorder. Current Protein and Peptide Science, 2007, 8, 173-179.	0.7	20
49	TOPDB: topology data bank of transmembrane proteins. Nucleic Acids Research, 2007, 36, D234-D239.	6.5	73
50	Local structural disorder imparts plasticity on linear motifs. Bioinformatics, 2007, 23, 950-956.	1.8	376
51	Molecular Principles of the Interactions of Disordered Proteins. Journal of Molecular Biology, 2007, 372, 549-561.	2.0	242
52	Electrostatic versus Nonelectrostatic Effects in DNA Sequence Discrimination by Divalent Ions Mg2+and Mn2+. Journal of Physical Chemistry B, 2007, 111, 6272-6279.	1.2	23
53	Impact of Ligand Protonation on Virtual Screening against Î²-Secretase (BACE1). Journal of Chemical Information and Modeling, 2007, 47, 2366-2373.	2.5	37
54	Probing the Two-Metal Ion Mechanism in the Restriction Endonuclease BamHI. Biochemistry, 2007, 46, 14514-14523.	1.2	27

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55	Metal-binding sites at the active site of restriction endonuclease BamHI can conform to a one-ion mechanism. Biological Chemistry, 2007, 388, 73-8.	1.2	10
56	An EcoRIâ€“RsrI chimeric restriction endonuclease retains parental sequence specificity. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2007, 1774, 583-594.	1.1	3
57	Disorder and Sequence Repeats in Hub Proteins and Their Implications for Network Evolution. Journal of Proteome Research, 2006, 5, 2985-2995.	1.8	312
58	Prevalent Structural Disorder inE.coliandS.cerevisiaeProteomes. Journal of Proteome Research, 2006, 5, 1996-2000.	1.8	119
59	Membrane topology of human ABC proteins. FEBS Letters, 2006, 580, 1017-1022.	1.3	70
60	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.	1.5	31
61	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
62	The BiSearch web server. BMC Bioinformatics, 2006, 7, 431.	1.2	86
63	Flexible segments modulate co-folding of dUTPase and nucleocapsid proteins. Nucleic Acids Research, 2006, 35, 495-505.	6.5	42
64	Flexibility of prolyl oligopeptidase: Molecular dynamics and molecular framework analysis of the potential substrate pathways. Proteins: Structure, Function and Bioinformatics, 2005, 60, 504-512.	1.5	51
65	TMDET: web server for detecting transmembrane regions of proteins by using their 3D coordinates. Bioinformatics, 2005, 21, 1276-1277.	1.8	132
66	BiSearch: primer-design and search tool for PCR on bisulfite-treated genomes. Nucleic Acids Research, 2005, 33, e9-e9.	6.5	159
67	IUPred: web server for the prediction of intrinsically unstructured regions of proteins based on estimated energy content. Bioinformatics, 2005, 21, 3433-3434.	1.8	1,832
68	SRide: a server for identifying stabilizing residues in proteins. Nucleic Acids Research, 2005, 33, W303-W305.	6.5	107
69	The Pairwise Energy Content Estimated from Amino Acid Composition Discriminates between Folded and Intrinsically Unstructured Proteins. Journal of Molecular Biology, 2005, 347, 827-839.	2.0	911
70	Interfacial Water as a â€œHydration Fingerprintâ€• in the Noncognate Complex of BamHI. Biophysical Journal, 2005, 89, 903-911.	0.2	49
71	PDB_TM: selection and membrane localization of transmembrane proteins in the protein data bank. Nucleic Acids Research, 2004, 33, D275-D278.	6.5	245
72	TM or not TM: transmembrane protein prediction with low false positive rate using DAS-TMfilter. Bioinformatics, 2004, 20, 136-137.	1.8	113

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73	Transmembrane proteins in the Protein Data Bank: identification and classification. Bioinformatics, 2004, 20, 2964-2972.	1.8	216
74	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.	1.5	73
75	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
76	Functionally and structurally relevant residues of enzymes: are they segregated or overlapping?. FEBS Letters, 2004, 567, 239-242.	1.3	8
77	Preformed Structural Elements Feature in Partner Recognition by Intrinsically Unstructured Proteins. Journal of Molecular Biology, 2004, 338, 1015-1026.	2.0	494
78	Servers for sequence-structure relationship analysis and prediction. Nucleic Acids Research, 2003, 31, 3359-3363.	6.5	12
79	SCide: identification of stabilization centers in proteins. Bioinformatics, 2003, 19, 899-900.	1.8	99
80	PSORT-B: improving protein subcellular localization prediction for Gram-negative bacteria. Nucleic Acids Research, 2003, 31, 3613-3617.	6.5	383
81	On filtering false positive transmembrane protein predictions. Protein Engineering, Design and Selection, 2002, 15, 745-752.	1.0	128
82	Predicting Redox State of Cysteines in Proteins. Methods in Enzymology, 2002, 353, 10-21.	0.4	13
83	Role of Base Flipping in Specific Recognition of Damaged DNA by Repair Enzymes. Journal of Molecular Biology, 2002, 323, 823-834.	2.0	64
84	The Role of Dimerization in Prion Replication. Biophysical Journal, 2002, 82, 1711-1718.	0.2	51
85	Modeling MHC class II molecules and their bound peptides as expressed at the cell surface. Molecular Immunology, 2002, 38, 681-687.	1.0	7
86	The role of hydrophobic microenvironments in modulating pKa shifts in proteins. Proteins: Structure, Function and Bioinformatics, 2002, 48, 283-292.	1.5	128
87	Role of stabilization centers in 4 helix bundle proteins. Proteins: Structure, Function and Bioinformatics, 2002, 48, 320-326.	1.5	14
88	Protein stability indicates divergent evolution of PD-(D/E)XK type II restriction endonucleases. Protein Science, 2002, 11, 1978-1983.	3.1	17
89	Topology of Membrane Proteins. Journal of Chemical Information and Computer Sciences, 2001, 41, 364-368.	2.8	37
90	Stabilization centers and protein stability. Theoretical Chemistry Accounts, 2001, 106, 121-127.	0.5	12

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91	Predicting protein conformation by statistical methods. BBA - Proteins and Proteomics, 2001, 1549, 123-136.	2.1	15
92	Prion protein: Evolution caught en route. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 4431-4436.	3.3	34
93	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.	1.8	24
94	Mapping of a Protective Helper T Cell Epitope of Human Influenza A Virus Hemagglutinin. Biochemical and Biophysical Research Communications, 2000, 270, 190-198.	1.0	14
95	Function-Related Regulation of the Stability of MHC Proteins. Biophysical Journal, 2000, 79, 2305-2313.	0.2	23
96	Stabilization centers in various proteins. Theoretical Chemistry Accounts, 1999, 101, 27-32.	0.5	8
97	Rod models of DNA: sequence-dependent anisotropic elastic modelling of local bending phenomena. Trends in Biochemical Sciences, 1998, 23, 341-347.	3.7	122
98	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.	2.0	1,023
99	The role of long-range interactions in defining the secondary structure of proteins is overestimated. Bioinformatics, 1997, 13, 297-301.	1.8	6
100	Stabilization centers in proteins:Identification, characterization and predictions. Journal of Molecular Biology, 1997, 272, 597-612.	2.0	144
101	The role of DNA bending in Cro protein-DNA interactions. Biophysical Chemistry, 1997, 69, 153-160.	1.5	19
102	Conservation of amino acids in multiple alignments: aspartic acid has unexpected conservation. FEBS Letters, 1996, 397, 225-229.	1.3	24
103	Repetitive elements of protein sequences as fossils of early life. Journal of Biological Physics, 1995, 20, 331-334.	0.7	0
104	Proteins as special subsets of polypeptides. Journal of Biosciences, 1995, 20, 579-590.	0.5	2
105	Independence divergence-generated binary trees of amino acids. Protein Engineering, Design and Selection, 1995, 8, 417-423.	1.0	5
106	Chaos game representation of protein structures. Journal of Molecular Graphics, 1994, 12, 302-304.	1.7	81
107	New Alignment Strategy for Transmembrane Proteins. Journal of Molecular Biology, 1994, 243, 388-396.	2.0	54
108	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

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109	Computation of low-energy crystalline arrangements of cellulose triacetate. Macromolecules, 1992, 25, 709-720.	2.2	22
110	Different sequence environments of cysteines and half cystines in proteins Application to predict disulfide forming residues. FEBS Letters, 1992, 302, 117-120.	1.3	58
111	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.	3.3	52
112	â€˜Rapid evolutionâ€™ of the amino acid composition of proteins. Trends in Biochemical Sciences, 1990, 15, 135-136.	3.7	18
113	Predicting isomorphic residue replacements for protein design. International Journal of Peptide and Protein Research, 1990, 36, 236-239.	0.1	31
114	Different segmental flexibility of human serum transferrin and lactoferrin. Archives of Biochemistry and Biophysics, 1989, 275, 181-184.	1.4	17
115	Structure of cellulose. 2. Low-energy crystalline arrangements. Macromolecules, 1988, 21, 990-998.	2.2	51
116	Structure of cellulose. 1. Low-energy conformations of single chains. Macromolecules, 1988, 21, 983-990.	2.2	38
117	A possible way for prediction of domain boundaries in globular proteins from amino acid sequence. Biochemical and Biophysical Research Communications, 1986, 139, 11-17.	1.0	40
118	Proteins as general crystals. Journal of Theoretical Biology, 1986, 123, 121-124.	0.8	5
119	Characteristic sequential residue environment of amino acids in proteins. International Journal of Peptide and Protein Research, 1986, 27, 483-492.	0.1	34
120	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.	0.8	2
121	Investigation of protein refolding: a special feature of native structure responsible for refolding ability. Journal of Theoretical Biology, 1985, 113, 703-710.	0.8	13
122	Conformation of human IgG subclasses in solution. Small-angle X-ray scattering and hydrodynamic studies. FEBS Journal, 1985, 147, 17-25.	0.2	63
123	The effect of iron binding on the conformation of transferrin. A small angle x-ray scattering study. Biophysical Journal, 1985, 48, 799-802.	0.2	66
124	Effect of trypsin binding on the hydrogen exchange kinetics of bovine pancreatic trypsin inhibitor .beta.-sheet NH's. Biochemistry, 1984, 23, 2064-2068.	1.2	14
125	Hydrogen exchange and the dynamic structure of proteins. Molecular and Cellular Biochemistry, 1982, 48, 135-160.	1.4	341
126	Possible mechanism for the dynamic stabilization of protein structure. Journal of Theoretical Biology, 1981, 90, 487-493.	0.8	2

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127	Subunit contact surfaceâ€"an additional argument in favour of continuous folding during biosynthesis of proteins. Journal of Theoretical Biology, 1980, 82, 685-688.	0.8	3
128	Investigation of protein folding: Uneven distribution of point mutations along polypeptide chains. Journal of Theoretical Biology, 1979, 81, 247-258.	0.8	5
129	Conformational Energy Calculations of the Effects of Sequence Variations on the Conformations of Two Tetrapeptides. Macromolecules, 1978, 11, 797-804.	2.2	48
130	Studies on the active center of pancreatic amylase. Molecular and Cellular Biochemistry, 1974, 4, 205-209.	1.4	28
131	Studies on the active center of pancreatic amylase. Molecular and Cellular Biochemistry, 1974, 4, 211-216.	1.4	16
132	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
133	Determination of small alterations in the radius of gyration by small-angle X-ray scattering. Journal of Applied Crystallography, 1971, 4, 317-318.	1.9	12