Istvan Simon

List of Publications by Year in Descending Order

131 papers	10,808 citations	47 h-index	103 g-index
137 ext. papers	11,742 ext. citations	5.9 avg, IF	6.19 L-index

#	Paper	IF	Citations
131	Sequential, Structural and Functional Properties of Protein Complexes Are Defined by How Folding and Binding Intertwine. *Journal of Molecular Biology*, **2019**, 431, 4408-4428	6.5	7
130	Analysis of Heterodimeric "Mutual Synergistic Folding"-Complexes. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	3
129	Bioinformatical Approaches to Unstructured/Disordered Proteins and Their Complexes. *Springer Series on Bio- and Neurosystems*, **2019**, 561-596	0.5	
128	DIBS: a repository of disordered binding sites mediating interactions with ordered proteins. *Bioinformatics*, **2018**, 34, 535-537	7.2	47
127	Physical Background of the Disordered Nature of "Mutual Synergetic Folding" Proteins. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	2
126	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	3.1	10
125	MFIB: a repository of protein complexes with mutual folding induced by binding. *Bioinformatics*, **2017**, 33, 3682-3684	7.2	41
124	Systematic analysis of somatic mutations driving cancer: uncovering functional protein regions in disease development. *Biology Direct*, **2016**, 11, 23	7.2	11
123	The role of stabilization centers in protein thermal stability. *Biochemical and Biophysical Research Communications*, **2016**, 471, 57-62	3.4	9
122	Combination of Pharmacophore Matching, 2D Similarity Search, and In Vitro Biological Assays in the Selection of Potential 5-HT6 Antagonists from Large Commercial Repositories. *Chemical Biology and Drug Design*, **2015**, 86, 864-80	2.9	5
121	Prediction and analysis of intrinsically disordered proteins. *Methods in Molecular Biology*, **2015**, 1261, 35-59	1.4	6
120	Self-regulating genes. Exact steady state solution by using Poisson representation. *Open Physics*, **2014**, 12,	1.3	4
119	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, 7008-39	4.8	17
118	A word of caution about biological inference - Revisiting cysteine covalent state predictions. *FEBS Open Bio*, **2014**, 4, 310-4	2.7	1
117	Bioinformatical Approaches to Unstructured/Disordered Proteins and Their Interactions. *Springer Series in Bio-/neuroinformatics*, **2014**, 525-556		1
116	Series of concentration-induced phase transitions in cholesterol/phosphatidylcholine mixtures. *Biophysical Journal*, **2013**, 104, 2448-55	2.9	4
115	PDBTM: Protein Data Bank of transmembrane proteins after 8 years. *Nucleic Acids Research*, **2013**, 41, D524-9	20.1	178

114	QM/MM simulation of liquid water with an adaptive quantum region. *Physical Chemistry Chemical Physics*, **2012**, 14, 646-56	3.6	74
113	Is there a biological cost of protein disorder? Analysis of cancer-associated mutations. *Molecular BioSystems*, **2012**, 8, 296-307		40
112	Disordered binding regions and linear motifs--bridging the gap between two models of molecular recognition. *PLoS ONE*, **2012**, 7, e46829	3.7	49
111	CMWeb: an interactive on-line tool for analysing residue-residue contacts and contact prediction methods. *Nucleic Acids Research*, **2012**, 40, W329-33	20.1	19
110	Active site residue involvement in monoamine or diamine oxidation catalysed by pea seedling amine oxidase. *FEBS Journal*, **2011**, 278, 1232-43	5.7	5
109	Dynamic protein-DNA recognition: beyond what can be seen. *Trends in Biochemical Sciences*, **2011**, 36, 415-23	10.3	116
108	The expanding view of protein-protein interactions: complexes involving intrinsically disordered proteins. *Physical Biology*, **2011**, 8, 035003	3	48
107	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, 14437-42	11.5	27
106	Proteins with complex architecture as potential targets for drug design: a case study of Mycobacterium tuberculosis. *PLoS Computational Biology*, **2011**, 7, e1002118	5	17
105	Bioinformatical approaches to characterize intrinsically disordered/unstructured proteins. *Briefings in Bioinformatics*, **2010**, 11, 225-43	13.4	99
104	Shedding Light on Transmembrane Topology **2010**, 107-135		1
103	Topology prediction of helical transmembrane proteins: how far have we reached?. *Current Protein and Peptide Science*, **2010**, 11, 550-61	2.8	27
102	Resource for structure related information on transmembrane proteins **2010**, 45-59		
101	ANCHOR: web server for predicting protein binding regions in disordered proteins. *Bioinformatics*, **2009**, 25, 2745-6	7.2	433
100	Prediction of protein binding regions in disordered proteins. *PLoS Computational Biology*, **2009**, 5, e1000376	5	419
99	EPIC-DB: a proteomics database for studying Apicomplexan organisms. *BMC Genomics*, **2009**, 10, 38	4.5	24
98	Close encounters of the third kind: disordered domains and the interactions of proteins. *BioEssays*, **2009**, 31, 328-35	4.1	197
97	Evaluating boundary dependent errors in QM/MM simulations. *Journal of Physical Chemistry B*, **2009** , 113, 5728-35	3.4	49

96	The energy gap as a universal reaction coordinate for the simulation of chemical reactions. *Journal of Physical Chemistry B*, **2009**, 113, 7867-73	3.4	34
95	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, 15084-5	16.4	53
94	Malleable machines take shape in eukaryotic transcriptional regulation. *Nature Chemical Biology*, **2008**, 4, 728-37	11.7	161
93	Substrate preference of transglutaminase 2 revealed by logistic regression analysis and intrinsic disorder examination. *Journal of Molecular Biology*, **2008**, 383, 390-402	6.5	29
92	Malleable machines in transcription regulation: the mediator complex. *PLoS Computational Biology*, **2008**, 4, e1000243	5	91
91	TOPDOM: database of domains and motifs with conservative location in transmembrane proteins. *Bioinformatics*, **2008**, 24, 1469-70	7.2	25
90	TOPDB: topology data bank of transmembrane proteins. *Nucleic Acids Research*, **2008**, 36, D234-9	20.1	65
89	Assessing Conservation of Disordered Regions in Proteins. *The Open Proteomics Journal*, **2008**, 1, 46-53		13
88	Impact of ligand protonation on virtual screening against beta-secretase (BACE1). *Journal of Chemical Information and Modeling*, **2007**, 47, 2366-73	6.1	34
87	Probing the two-metal ion mechanism in the restriction endonuclease BamHI. *Biochemistry*, **2007**, 46, 14514-23	3.2	24
86	Metal-binding sites at the active site of restriction endonuclease BamHI can conform to a one-ion mechanism. *Biological Chemistry*, **2007**, 388, 73-8	4.5	9
85	An EcoRI-RsrI chimeric restriction endonuclease retains parental sequence specificity. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2007**, 1774, 583-94	4	3
84	Flexible segments modulate co-folding of dUTPase and nucleocapsid proteins. *Nucleic Acids Research*, **2007**, 35, 495-505	20.1	40
83	Prediction of protein disorder at the domain level. *Current Protein and Peptide Science*, **2007**, 8, 161-71	2.8	65
82	Towards proteomic approaches for the identification of structural disorder. *Current Protein and Peptide Science*, **2007**, 8, 173-9	2.8	16
81	Local structural disorder imparts plasticity on linear motifs. *Bioinformatics*, **2007**, 23, 950-6	7.2	335
80	Molecular principles of the interactions of disordered proteins. *Journal of Molecular Biology*, **2007**, 372, 549-61	6.5	220
79	Electrostatic versus nonelectrostatic effects in DNA sequence discrimination by divalent ions Mg2+ and Mn2+. *Journal of Physical Chemistry B*, **2007**, 111, 6272-9	3.4	23

78	The BiSearch web server. *BMC Bioinformatics*, **2006**, 7, 431	3.6	74
77	Disorder and sequence repeats in hub proteins and their implications for network evolution. *Journal of Proteome Research*, **2006**, 5, 2985-95	5.6	273
76	Prevalent structural disorder in E. coli and S. cerevisiae proteomes. *Journal of Proteome Research*, **2006**, 5, 1996-2000	5.6	102
75	Membrane topology of human ABC proteins. *FEBS Letters*, **2006**, 580, 1017-22	3.8	66
74	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, 749-57	4.2	27
73	Molecular dynamics approach to study the discrepancies in the thermal behavior of amylose and chitosan conformations. *Computational and Theoretical Chemistry*, **2006**, 764, 133-140		15
72	The pairwise energy content estimated from amino acid composition discriminates between folded and intrinsically unstructured proteins. *Journal of Molecular Biology*, **2005**, 347, 827-39	6.5	767
71	Interfacial water as a "hydration fingerprint" in the noncognate complex of BamHI. *Biophysical Journal*, **2005**, 89, 903-11	2.9	49
70	PDB_TM: selection and membrane localization of transmembrane proteins in the protein data bank. *Nucleic Acids Research*, **2005**, 33, D275-8	20.1	221
69	Flexibility of prolyl oligopeptidase: molecular dynamics and molecular framework analysis of the potential substrate pathways. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 504-12	4.2	49
68	TMDET: web server for detecting transmembrane regions of proteins by using their 3D coordinates. *Bioinformatics*, **2005**, 21, 1276-7	7.2	116
67	BiSearch: primer-design and search tool for PCR on bisulfite-treated genomes. *Nucleic Acids Research*, **2005**, 33, e9	20.1	137
66	IUPred: web server for the prediction of intrinsically unstructured regions of proteins based on estimated energy content. *Bioinformatics*, **2005**, 21, 3433-4	7.2	1571
65	SRide: a server for identifying stabilizing residues in proteins. *Nucleic Acids Research*, **2005**, 33, W303-5	20.1	95
64	TM or not TM: transmembrane protein prediction with low false positive rate using DAS-TMfilter. *Bioinformatics*, **2004**, 20, 136-7	7.2	89
63	Transmembrane proteins in the Protein Data Bank: identification and classification. *Bioinformatics*, **2004**, 20, 2964-72	7.2	188
62	Locating the stabilizing residues in (alpha/beta)8 barrel proteins based on hydrophobicity, long-range interactions, and sequence conservation. *Proteins: Structure, Function and Bioinformatics* , **2004**, 55, 316-29	4.2	65
61	Noncovalent cross-links in context with other structural and functional elements of proteins. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 347-51		4

60	Functionally and structurally relevant residues of enzymes: are they segregated or overlapping?. *FEBS Letters*, **2004**, 567, 239-42	3.8	6
59	Preformed structural elements feature in partner recognition by intrinsically unstructured proteins. *Journal of Molecular Biology*, **2004**, 338, 1015-26	6.5	448
58	Servers for sequence-structure relationship analysis and prediction. *Nucleic Acids Research*, **2003**, 31, 3359-63	20.1	10
57	SCide: identification of stabilization centers in proteins. *Bioinformatics*, **2003**, 19, 899-900	7.2	87
56	PSORT-B: Improving protein subcellular localization prediction for Gram-negative bacteria. *Nucleic Acids Research*, **2003**, 31, 3613-7	20.1	318
55	The role of hydrophobic microenvironments in modulating pKa shifts in proteins. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 283-92	4.2	116
54	Role of stabilization centers in 4 helix bundle proteins. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 320-6	4.2	11
53	Protein stability indicates divergent evolution of PD-(D/E)XK type II restriction endonucleases. *Protein Science*, **2002**, 11, 1978-83	6.3	14
52	On filtering false positive transmembrane protein predictions. *Protein Engineering, Design and Selection*, **2002**, 15, 745-52	1.9	119
51	Predicting redox state of cysteines in proteins. *Methods in Enzymology*, **2002**, 353, 10-21	1.7	12
50	Role of base flipping in specific recognition of damaged DNA by repair enzymes. *Journal of Molecular Biology*, **2002**, 323, 823-34	6.5	59
49	The role of dimerization in prion replication. *Biophysical Journal*, **2002**, 82, 1711-8	2.9	44
48	Modeling MHC class II molecules and their bound peptides as expressed at the cell surface. *Molecular Immunology*, **2002**, 38, 681-7	4.3	6
47	Stabilization centers and protein stability. *Theoretical Chemistry Accounts*, **2001**, 106, 121-127	1.9	12
46	Predicting protein conformation by statistical methods. *BBA - Proteins and Proteomics*, **2001**, 1549, 123-36		13
45	Prion protein: evolution caught en route. *Proceedings of the National Academy of Sciences of the United States of America*, **2001**, 98, 4431-6	11.5	31
44	Topology of membrane proteins. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 364-8		32
43	A repetitive sequence of Epstein-Barr virus nuclear antigen 6 comprises overlapping T cell epitopes which induce HLA-DR-restricted CD4(+) T lymphocytes. *International Immunology*, **2000**, 12, 281-93	4.9	19

42	Mapping of a protective helper T cell epitope of human influenza A virus hemagglutinin. *Biochemical and Biophysical Research Communications*, **2000**, 270, 190-8	3.4	13
41	Function-related regulation of the stability of MHC proteins. *Biophysical Journal*, **2000**, 79, 2305-13	2.9	22
40	Stabilization centers in various proteins. *Theoretical Chemistry Accounts*, **1999**, 101, 27-32	1.9	8
39	Rod models of DNA: sequence-dependent anisotropic elastic modelling of local bending phenomena. *Trends in Biochemical Sciences*, **1998**, 23, 341-7	10.3	114
38	Principles governing amino acid composition of integral membrane proteins: application to topology prediction. *Journal of Molecular Biology*, **1998**, 283, 489-506	6.5	934
37	The role of long-range interactions in defining the secondary structure of proteins is overestimated. *Bioinformatics*, **1997**, 13, 297-301	7.2	5
36	Stabilization centers in proteins: identification, characterization and predictions. *Journal of Molecular Biology*, **1997**, 272, 597-612	6.5	130
35	The role of DNA bending in Cro protein-DNA interactions. *Biophysical Chemistry*, **1997**, 69, 153-60	3.5	19
34	Conservation of amino acids in multiple alignments: aspartic acid has unexpected conservation. *FEBS Letters*, **1996**, 397, 225-9	3.8	19
33	Repetitive elements of protein sequences as fossils of early life. *Journal of Biological Physics*, **1995**, 20, 331-334	1.6	
32	Proteins as special subsets of polypeptides. *Journal of Biosciences*, **1995**, 20, 579-590	2.3	2
31	Independence divergence-generated binary trees of amino acids. *Protein Engineering, Design and Selection*, **1995**, 8, 417-23	1.9	5
30	Different sequence environments of amino acid residues involved and not involved in long-range interactions in proteins. *International Journal of Peptide and Protein Research*, **1994**, 43, 205-8		13
29	Chaos game representation of protein structures. *Journal of Molecular Graphics*, **1994**, 12, 302-4, 295		49
28	New alignment strategy for transmembrane proteins. *Journal of Molecular Biology*, **1994**, 243, 388-96	6.5	53
27	Computation of low-energy crystalline arrangements of cellulose triacetate. *Macromolecules*, **1992**, 25, 709-720	5.5	21
26	Different sequence environments of cysteines and half cystines in proteins. Application to predict disulfide forming residues. *FEBS Letters*, **1992**, 302, 117-20	3.8	48
25	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, 3661-5	11.5	47

24	Predicting isomorphic residue replacements for protein design. *International Journal of Peptide and Protein Research*, **1990**, 36, 236-9		29
23	Rapid evolution of the amino acid composition of proteins. *Trends in Biochemical Sciences*, **1990**, 15, 135-6	10.3	18
22	Regularities in the primary structure of proteins. *International Journal of Peptide and Protein Research*, **1989**, 34, 184-95		29
21	Different segmental flexibility of human serum transferrin and lactoferrin. *Archives of Biochemistry and Biophysics*, **1989**, 275, 181-4	4.1	15
20	Structure of cellulose. 2. Low-energy crystalline arrangements. *Macromolecules*, **1988**, 21, 990-998	5.5	43
19	Structure of cellulose. 1. Low-energy conformations of single chains. *Macromolecules*, **1988**, 21, 983-990	5.5	32
18	Characteristic sequential residue environment of amino acids in proteins. *International Journal of Peptide and Protein Research*, **1986**, 27, 483-92		31
17	Proteins as general crystals. *Journal of Theoretical Biology*, **1986**, 123, 121-4	2.3	5
16	A possible way for prediction of domain boundaries in globular proteins from amino acid sequence. *Biochemical and Biophysical Research Communications*, **1986**, 139, 11-7	3.4	37
15	Electrostatic effect of trypsin binding on the hydrogen exchange rate of bovine pancreatic trypsin inhibitor beta-sheet NHs. *Journal of Theoretical Biology*, **1985**, 117, 505-8	2.3	1
14	Investigation of protein refolding: a special feature of native structure responsible for refolding ability. *Journal of Theoretical Biology*, **1985**, 113, 703-10	2.3	12
13	Conformation of human IgG subclasses in solution. Small-angle X-ray scattering and hydrodynamic studies. *FEBS Journal*, **1985**, 147, 17-25		55
12	The effect of iron binding on the conformation of transferrin. A small angle x-ray scattering study. *Biophysical Journal*, **1985**, 48, 799-802	2.9	63
11	Effect of trypsin binding on the hydrogen exchange kinetics of bovine pancreatic trypsin inhibitor .beta.-sheet NHs. *Biochemistry*, **1984**, 23, 2064-2068	3.2	11
10	Hydrogen exchange and the dynamic structure of proteins. *Molecular and Cellular Biochemistry*, **1982**, 48, 135-60	4.2	302
9	Possible mechanism for the dynamic stabilization of protein structure. *Journal of Theoretical Biology*, **1981**, 90, 487-93	2.3	2
8	Subunit contact surface--an additional argument in favour of continuous folding during biosynthesis of proteins. *Journal of Theoretical Biology*, **1980**, 82, 685-8	2.3	3
7	Investigation of protein folding: uneven distribution of point mutations along polypeptide chains. *Journal of Theoretical Biology*, **1979**, 81, 247-58	2.3	5

6	Conformational Energy Calculations of the Effects of Sequence Variations on the Conformations of Two Tetrapeptides. *Macromolecules*, **1978**, 11, 797-804	5.5	42
5	Studies on the active center of pancreatic amylase. I. Binding of beta-cyclodextrin. *Molecular and Cellular Biochemistry*, **1974**, 4, 205-9	4.2	25
4	Studies on the active center of pancreatic amylase. II. Small angle x-ray scattering investigations. *Molecular and Cellular Biochemistry*, **1974**, 4, 211-6	4.2	13
3	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, 184-9		25
2	Determination of small alterations in the radius of gyration by small-angle X-ray scattering. *Journal of Applied Crystallography*, **1971**, 4, 317-318	3.8	12
1	Interplay between folding and binding modulates protein sequences, structures, functions and regulation		1