Werner Braun

List of Publications by Citations

105 papers	7,994 citations	42 h-index	89 g-index
107 ext. papers	8,444 ext. citations	5.2 avg, IF	5.6 L-index

#	Paper	IF	Citations
105	Efficient computation of three-dimensional protein structures in solution from nuclear magnetic resonance data using the program DIANA and the supporting programs CALIBA, HABAS and GLOMSA. *Journal of Molecular Biology*, **1991**, 217, 517-30	6.5	864
104	Exact and efficient analytical calculation of the accessible surface areas and their gradients for macromolecules. *Journal of Computational Chemistry*, **1998**, 19, 319-333	3.5	802
103	Polypeptide secondary structure determination by nuclear magnetic resonance observation of short proton-proton distances. *Journal of Molecular Biology*, **1984**, 180, 715-40	6.5	658
102	Protein structures in solution by nuclear magnetic resonance and distance geometry. The polypeptide fold of the basic pancreatic trypsin inhibitor determined using two different algorithms, DISGEO and DISMAN. *Journal of Molecular Biology*, **1987**, 196, 611-39	6.5	596
101	Sequential resonance assignments as a basis for determination of spatial protein structures by high resolution proton nuclear magnetic resonance. *Journal of Molecular Biology*, **1982**, 155, 311-9	6.5	488
100	Three-dimensional structure of rabbit liver [Cd7]metallothionein-2a in aqueous solution determined by nuclear magnetic resonance. *Journal of Molecular Biology*, **1988**, 201, 637-57	6.5	275
99	Determination of the complete three-dimensional structure of the alpha-amylase inhibitor tendamistat in aqueous solution by nuclear magnetic resonance and distance geometry. *Journal of Molecular Biology*, **1988**, 204, 675-724	6.5	208
98	SDAP: database and computational tools for allergenic proteins. *Nucleic Acids Research*, **2003**, 31, 359-62	20.1	188
97	Distance geometry and related methods for protein structure determination from NMR data. *Quarterly Reviews of Biophysics*, **1987**, 19, 115-57	7	181
96	Measles virus blind to its epithelial cell receptor remains virulent in rhesus monkeys but cannot cross the airway epithelium and is not shed. *Journal of Clinical Investigation*, **2008**, 118, 2448-58	15.9	169
95	Selectively receptor-blind measles viruses: Identification of residues necessary for SLAM- or CD46-induced fusion and their localization on a new hemagglutinin structural model. *Journal of Virology*, **2004**, 78, 302-13	6.6	164
94	Comparison of the high-resolution structures of the alpha-amylase inhibitor tendamistat determined by nuclear magnetic resonance in solution and by X-ray diffraction in single crystals. *Journal of Molecular Biology*, **1989**, 206, 677-87	6.5	148
93	New quantitative descriptors of amino acids based on multidimensional scaling of a large number of physical□hemical properties. *Journal of Molecular Modeling*, **2001**, 7, 445-453	2	136
92	Polypeptide fold in the two metal clusters of metallothionein-2 by nuclear magnetic resonance in solution. *Journal of Molecular Biology*, **1986**, 187, 125-9	6.5	133
91	Automated combined assignment of NOESY spectra and three-dimensional protein structure determination. *Journal of Biomolecular NMR*, **1997**, 10, 351-62	3	128
90	InterProSurf: a web server for predicting interacting sites on protein surfaces. *Bioinformatics*, **2007**, 23, 3397-9	7.2	126
89	Efficient search for all low energy conformations of polypeptides by Monte Carlo methods. *Journal of Computational Chemistry*, **1991**, 12, 1065-1076	3.5	98

88	Cyclosporin A-cyclophilin complex formation. A model based on X-ray and NMR data. *FEBS Letters*, **1992**, 300, 291-300	3.8	85
87	The heads of the measles virus attachment protein move to transmit the fusion-triggering signal. *Nature Structural and Molecular Biology*, **2011**, 18, 128-34	17.6	84
86	Three-dimensional structure and actions of immunosuppressants and their immunophilins. *FASEB Journal*, **1995**, 9, 63-72	0.9	79
85	The program FANTOM for energy refinement of polypeptides and proteins using a Newton Raphson minimizer in torsion angle space. *Biopolymers*, **1990**, 29, 679-694	2.2	79
84	Mapping of the primary binding site of measles virus to its receptor CD46. *Journal of Biological Chemistry*, **1997**, 272, 22072-9	5.4	74
83	Bioinformatics approaches to classifying allergens and predicting cross-reactivity. *Immunology and Allergy Clinics of North America*, **2007**, 27, 1-27	3.3	73
82	Data mining of sequences and 3D structures of allergenic proteins. *Bioinformatics*, **2002**, 18, 1358-64	7.2	73
81	Host S-nitrosylation inhibits clostridial small molecule-activated glucosylating toxins. *Nature Medicine*, **2011**, 17, 1136-41	50.5	67
80	Homology modeling and characterization of IgE binding epitopes of mountain cedar allergen Jun a 3. *Biophysical Journal*, **2000**, 79, 1601-9	2.9	66
79	Characteristic motifs for families of allergenic proteins. *Molecular Immunology*, **2009**, 46, 559-68	4.3	65
78	Conformational flexibility of mammalian cytochrome P450 2B4 in binding imidazole inhibitors with different ring chemistry and side chains. Solution thermodynamics and molecular modeling. *Journal of Biological Chemistry*, **2006**, 281, 8051-61	5.4	64
77	Exact and efficient analytical calculation of the accessible surface areas and their gradients for macromolecules **1998**, 19, 319		61
76	Automated detection of conformational epitopes using phage display Peptide sequences. *Bioinformatics and Biology Insights*, **2009**, 3, 71-81	5.3	60
75	Comprehensive 3D-modeling of allergenic proteins and amino acid composition of potential conformational IgE epitopes. *Molecular Immunology*, **2008**, 45, 3740-7	4.3	60
74	Nearby clusters of hemagglutinin residues sustain SLAM-dependent canine distemper virus entry in peripheral blood mononuclear cells. *Journal of Virology*, **2005**, 79, 5857-62	6.6	58
73	Dynamic interaction of the measles virus hemagglutinin with its receptor signaling lymphocytic activation molecule (SLAM, CD150). *Journal of Biological Chemistry*, **2008**, 283, 11763-71	5.4	57
72	Structural and functional analysis of Aplysia attractins, a family of water-borne protein pheromones with interspecific attractiveness. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 6929-33	11.5	52
71	A "moving metal mechanism" for substrate cleavage by the DNA repair endonuclease APE-1. *Proteins: Structure, Function and Bioinformatics*, **2007**, 68, 313-23	4.2	51

70	Sequence specificity, statistical potentials, and three-dimensional structure prediction with self-correcting distance geometry calculations of beta-sheet formation in proteins. *Protein Science*, **1999**, 8, 326-42	6.3	51
69	Minimization of empirical energy functions in proteins including hydrophobic surface area effects. *Journal of Computational Chemistry*, **1993**, 14, 510-521	3.5	51
68	Detecting potential IgE-reactive sites on food proteins using a sequence and structure database, SDAP-food. *Journal of Agricultural and Food Chemistry*, **2003**, 51, 4830-7	5.7	49
67	Surface area included in energy refinement of proteins. A comparative study on atomic solvation parameters. *Journal of Molecular Biology*, **1993**, 233, 275-92	6.5	48
66	Extensive distance geometry calculations with different NOE calibrations: new criteria for structure selection applied to Sandostatin and BPTI. *Journal of Biomolecular NMR*, **1993**, 3, 307-24	3	44
65	Membrane fusion triggering: three modules with different structure and function in the upper half of the measles virus attachment protein stalk. *Journal of Biological Chemistry*, **2012**, 287, 38543-51	5.4	43
64	Using property based sequence motifs and 3D modeling to determine structure and functional regions of proteins. *Current Medicinal Chemistry*, **2004**, 11, 583-93	4.3	43
63	The property distance index PD predicts peptides that cross-react with IgE antibodies. *Molecular Immunology*, **2009**, 46, 873-83	4.3	42
62	Membrane-protein interactions contribute to efficient 27-hydroxylation of cholesterol by mitochondrial cytochrome P450 27A1. *Journal of Biological Chemistry*, **2002**, 277, 37582-9	5.4	42
61	Major linear IgE epitopes of mountain cedar pollen allergen Jun a 1 map to the pectate lyase catalytic site. *Molecular Immunology*, **2003**, 40, 555-62	4.3	41
60	1H nuclear-magnetic-resonance studies of the three-dimensional structure of the cardiotoxin CTXIIb from Naja mossambica mossambica in aqueous solution and comparison with the crystal structures of homologous toxins. *FEBS Journal*, **1988**, 172, 101-16		39
59	Common physical-chemical properties correlate with similar structure of the IgE epitopes of peanut allergens. *Journal of Agricultural and Food Chemistry*, **2005**, 53, 8752-9	5.7	37
58	Aplysia attractin: biophysical characterization and modeling of a water-borne pheromone. *Biophysical Journal*, **2001**, 81, 463-72	2.9	37
57	Complete relaxation matrix refinement of NMR structures of proteins using analytically calculated dihedral angle derivatives of NOE intensities. *Journal of Biomolecular NMR*, **1991**, 1, 257-69	3	37
56	Conformational polymorphism of cyclosporin A. *Structure*, **1994**, 2, 963-72	5.2	36
55	NMR structure of the viral peptide linked to the genome (VPg) of poliovirus. *Peptides*, **2006**, 27, 1676-84	3.8	35
54	Identifying property based sequence motifs in protein families and superfamilies: application to DNase-1 related endonucleases. *Bioinformatics*, **2003**, 19, 1381-90	7.2	35
53	Base of the measles virus fusion trimer head receives the signal that triggers membrane fusion. *Journal of Biological Chemistry*, **2012**, 287, 33026-35	5.4	34

52	Statistical analysis of physical-chemical properties and prediction of protein-protein interfaces. *Journal of Molecular Modeling*, **2007**, 13, 1157-67	2	32
51	Unusual role of a cysteine residue in substrate binding and activity of human AP-endonuclease 1. *Journal of Molecular Biology*, **2008**, 379, 28-37	6.5	31
50	Conformational IgE epitopes of peanut allergens Ara h 2 and Ara h 6. *Clinical and Experimental Allergy*, **2016**, 46, 1120-1128	4.1	30
49	Molluscan attractins, a family of water-borne protein pheromones with interspecific attractiveness. *Peptides*, **2005**, 26, 121-9	3.8	29
48	Structural basis for epitope sharing between group 1 allergens of cedar pollen. *Molecular Immunology*, **2006**, 43, 509-18	4.3	29
47	Structural analysis of linear and conformational epitopes of allergens. *Regulatory Toxicology and Pharmacology*, **2009**, 54, S11-9	3.4	27
46	Molego-based definition of the architecture and specificity of metal-binding sites. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 200-10	4.2	26
45	Effects of backbone contacts 3Sto the abasic site on the cleavage and the product binding by human apurinic/apyrimidinic endonuclease (APE1). *Biochemistry*, **2004**, 43, 684-9	3.2	26
44	Formulation of Static and Dynamic Conformational Energy Analysis of Biopolymer Systems Consisting of Two or More Molecules. *Journal of the Physical Society of Japan*, **1984**, 53, 3269-3275	1.5	26
43	Representation of short and long-range handedness in protein structures by signed distance maps. *Journal of Molecular Biology*, **1983**, 163, 613-21	6.5	23
42	A 3D model for the measles virus receptor CD46 based on homology modeling, Monte Carlo simulations, and hemagglutinin binding studies. *Protein Science*, **1997**, 6, 588-97	6.3	22
41	Automated assignment and 3D structure calculations using combinations of 2D homonuclear and 3D heteronuclear NOESY spectra. *Journal of Biomolecular NMR*, **2002**, 22, 249-63	3	21
40	Determining functionally important amino acid residues of the E1 protein of Venezuelan equine encephalitis virus. *Journal of Molecular Modeling*, **2006**, 12, 921-9	2	20
39	Mechanical stability and differentially conserved physical-chemical properties of titin Ig-domains. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 706-18	4.2	19
38	Robust quantitative modeling of peptide binding affinities for MHC molecules using physical-chemical descriptors. *Protein and Peptide Letters*, **2007**, 14, 903-16	1.9	19
37	Total sequence decomposition distinguishes functional modules, "molegos" in apurinic/apyrimidinic endonucleases. *BMC Bioinformatics*, **2002**, 3, 37	3.6	18
36	An Allergen Portrait Gallery: Representative Structures and an Overview of IgE Binding Surfaces. *Bioinformatics and Biology Insights*, **2010**, 4, 113-25	5.3	16
35	Stereophysicochemical variability plots highlight conserved antigenic areas in Flaviviruses. *Virology Journal*, **2005**, 2, 40	6.1	16

34	Validation of a phage display and computational algorithm by mapping a conformational epitope of Bla g 2. *International Archives of Allergy and Immunology*, **2012**, 157, 323-30	3.7	15
33	Homology modeling and simulations of nuclease structures. *Methods in Molecular Biology*, **2001**, 160, 263-86	1.4	15
32	NMR solution structure of poliovirus uridylyated peptide linked to the genome (VPgpU). *Peptides*, **2010**, 31, 1441-8	3.8	14
31	MD simulation and experimental evidence for Mg□+ binding at the B site in human AP endonuclease 1. *Bioinformation*, **2011**, 7, 184-98	1.1	14
30	The importance of the 2S albumins for allergenicity and cross-reactivity of peanuts, tree nuts, and sesame seeds. *Journal of Allergy and Clinical Immunology*, **2021**, 147, 1154-1163	11.5	14
29	Distinguishing allergens from non-allergenic homologues using Physical-Chemical Property (PCP) motifs. *Molecular Immunology*, **2018**, 99, 1-8	4.3	13
28	IgE binding to linear epitopes of Ara h 2 in peanut allergic preschool children undergoing oral Immunotherapy. *Pediatric Allergy and Immunology*, **2019**, 30, 817-823	4.2	13
27	Assessment of 3D models for allergen research. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 545-54	4.2	13
26	Identification and analysis of conserved sequence motifs in cytochrome P450 family 2. Functional and structural role of a motif 187RFDYKD192 in CYP2B enzymes. *Journal of Biological Chemistry*, **2008**, 283, 21808-16	5.4	12
25	Functional classification of protein toxins as a basis for bioinformatic screening. *Scientific Reports*, **2017**, 7, 13940	4.9	11
24	A multimeric model for murine anti-apoptotic protein Bcl-2 and structural insights for its regulation by post-translational modification. *Journal of Molecular Modeling*, **2003**, 9, 298-303	2	11
23	Co-localization of glyceraldehyde-3-phosphate dehydrogenase with ferredoxin-NADP reductase in pea leaf chloroplasts. *Journal of Structural Biology*, **2008**, 161, 18-30	3.4	9
22	Conformational studies of cyclic peptide structures in solution from 1H-Nmr data by distance geometry calculation and restrained energy minimization. *Biopolymers*, **1990**, 29, 1387-400	2.2	9
21	Cross-React: a new structural bioinformatics method for predicting allergen cross-reactivity. *Bioinformatics*, **2017**, 33, 1014-1020	7.2	8
20	Engineering proteins with enhanced mechanical stability by force-specific sequence motifs. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1308-15	4.2	8
19	AllerML: markup language for allergens. *Regulatory Toxicology and Pharmacology*, **2011**, 60, 151-60	3.4	8
18	Homology Modeling and Molecular Dynamics Simulations of PBCV-1 Glycosylase Complexed with UV-damaged DNA. *Journal of Molecular Modeling*, **1999**, 5, 302-316	2	8
17	Novel neutralizing monoclonal antibodies protect rodents against lethal filovirus challenges. *Trials in Vaccinology*, **2014**, 3, 89-94		7

16	Membrane interaction and functional plasticity of inositol polyphosphate 5-phosphatases. *Structure* , **2014**, 22, 664-6	5.2	7
15	Clostridial toxins: sensing a target in a hostile gut environment. *Gut Microbes*, **2012**, 3, 35-41	8.8	6
14	A Conserved Structural Signature of the Homeobox Coding DNA in HOX genes. *Scientific Reports*, **2016**, 6, 35415	4.9	6
13	Antibody-Mediated Protective Mechanisms Induced by a Trivalent Parainfluenza Virus-Vectored Ebolavirus Vaccine. *Journal of Virology*, **2019**, 93,	6.6	6
12	Regional and temporal coordinated mutation patterns in SARS-CoV-2 spike protein revealed by a clustering and network analysis.. *Scientific Reports*, **2022**, 12, 1128	4.9	5
11	Conformational flexibility of mammalian cytochrome P450 2B4 in binding imidazole inhibitors of different ring chemistry and side chains. *FASEB Journal*, **2006**, 20, A264	0.9	4
10	Producing physicochemical property consensus alphavirus protein antigens for broad spectrum vaccine design. *Antiviral Research*, **2020**, 182, 104905	10.8	4
9	Determining the three-dimensional fold of a protein from approximate constraints: a simulation study. *Cell Biochemistry and Biophysics*, **2001**, 34, 283-304	3.2	3
8	DGraph Clusters Flaviviruses and Coronaviruses According to Their Hosts, Disease Type, and Human Cell Receptors. *Bioinformatics and Biology Insights*, **2021**, 15, 11779322211020316	5.3	3
7	Synthetic proteins for COVID-19 diagnostics. *Peptides*, **2021**, 143, 170583	3.8	2
6	D-graph clusters flaviviruses and coronaviruses according to their hosts, disease type and human cell receptors **2020**,		1
5	Exact and efficient analytical calculation of the accessible surface areas and their gradients for macromolecules **1998**, 19, 319		1
4	Designing multivalent immunogens for alphavirus vaccine optimization. *Virology*, **2021**, 561, 117-124	3.6	0
3	Developing computational tools for NMR: the early days of protein NMR. *Magnetic Resonance in Chemistry*, **2003**, 41, S51-S55	2.1	
2	Design of peptides with high affinity binding to a monoclonal antibody as a basis for immunotherapy. *Peptides*, **2021**, 145, 170628	3.8	
1	Still SDAPing Along: 20 Years of the Structural Database of Allergenic Proteins.. *Frontiers in Allergy*, **2022**, 3, 863172	0	