

Thomas Huber

List of Publications by Year in descending order

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111
papers

18,204
citations

57758

44
h-index

23533

111
g-index

119
all docs

119
docs citations

119
times ranked

25774
citing authors

#	ARTICLE	IF	CITATIONS
1	Greengenes, a Chimera-Checked 16S rRNA Gene Database and Workbench Compatible with ARB. Applied and Environmental Microbiology, 2006, 72, 5069-5072.	3.1	9,859
2	Bellerophon: a program to detect chimeric sequences in multiple sequence alignments. Bioinformatics, 2004, 20, 2317-2319.	4.1	1,443
3	The GROMOS Biomolecular Simulation Program Package. Journal of Physical Chemistry A, 1999, 103, 3596-3607.	2.5	1,354
4	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
5	Local elevation: A method for improving the searching properties of molecular dynamics simulation. Journal of Computer-Aided Molecular Design, 1994, 8, 695-708.	2.9	510
6	Chimeric 16S rDNA sequences of diverse origin are accumulating in the public databases. International Journal of Systematic and Evolutionary Microbiology, 2003, 53, 289-293.	1.7	203
7	Numbat: an interactive software tool for fitting $\hat{\Gamma}^{\text{H}}\hat{\Gamma}^{\text{H}}$ -tensors to molecular coordinates using pseudocontact shifts. Journal of Biomolecular NMR, 2008, 41, 179-189.	2.8	168
8	Nanometer-Scale Distance Measurements in Proteins Using Gd ³⁺ Spin Labeling. Journal of the American Chemical Society, 2010, 132, 9040-9048.	13.7	143
9	Structure refinement using time-averaged J-coupling constant restraints. Journal of Biomolecular NMR, 1993, 3, 55-66.	2.8	125
10	Binding of Low Molecular Weight Inhibitors Promotes Large Conformational Changes in the Dengue Virus NS2B-NS3 Protease: Fold Analysis by Pseudocontact Shifts. Journal of the American Chemical Society, 2011, 133, 19205-19215.	13.7	119
11	A Dipicolinic Acid Tag for Rigid Lanthanide Tagging of Proteins and Paramagnetic NMR Spectroscopy. Journal of the American Chemical Society, 2008, 130, 10486-10487.	13.7	117
12	Protein Structure Determination from Pseudocontact Shifts Using ROSETTA. Journal of Molecular Biology, 2012, 416, 668-677.	4.2	106
13	DOTA-Amide Lanthanide Tag for Reliable Generation of Pseudocontact Shifts in Protein NMR Spectra. Bioconjugate Chemistry, 2011, 22, 2118-2125.	3.6	104
14	Gadolinium Tagging for High-Precision Measurements of 6 nm Distances in Protein Assemblies by EPR. Journal of the American Chemical Society, 2011, 133, 10418-10421.	13.7	104
15	Lanthanide-Binding Peptides for NMR Measurements of Residual Dipolar Couplings and Paramagnetic Effects from Multiple Angles. Journal of the American Chemical Society, 2008, 130, 1681-1687.	13.7	96
16	3D structure determination of a protein in living cells using paramagnetic NMR spectroscopy. Chemical Communications, 2016, 52, 10237-10240.	4.1	90
17	Systematic Characterization of the Zinc-Finger-Containing Proteins in the Mouse Transcriptome. Genome Research, 2003, 13, 1430-1442.	5.5	89
18	Multiple- ϵ -Site Labeling of Proteins with Unnatural Amino Acids. Angewandte Chemie - International Edition, 2012, 51, 2243-2246.	13.8	89

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19	A direct proofreaderâ€™clamp interaction stabilizes the Pol III replicase in the polymerization mode. EMBO Journal, 2013, 32, 1322-1333.	7.8	85
20	Fast Structure-Based Assignment of ¹⁵ N HSQC Spectra of Selectively ¹⁵ N-Labeled Paramagnetic Proteins. Journal of the American Chemical Society, 2004, 126, 2963-2970.	13.7	83
21	Prediction of cis/trans isomerization in proteins using PSI-BLAST profiles and secondary structure information. BMC Bioinformatics, 2006, 7, 124.	2.6	83
22	Site-Specific Labelling of Proteins with a Rigid Lanthanide-Binding Tag. ChemBioChem, 2006, 7, 1599-1604.	2.6	82
23	Lanthanide Tags for Site-Specific Ligation to an Unnatural Amino Acid and Generation of Pseudocontact Shifts in Proteins. Bioconjugate Chemistry, 2013, 24, 260-268.	3.6	81
24	Three-Dimensional Protein Fold Determination from Backbone Amide Pseudocontact Shifts Generated by Lanthanide Tags at Multiple Sites. Structure, 2013, 21, 883-890.	3.3	77
25	Spectroscopic selection of distance measurements in a protein dimer with mixed nitroxide and Gd ³⁺ spin labels. Physical Chemistry Chemical Physics, 2012, 14, 4355.	2.8	73
26	Nanometer-Range Distance Measurement in a Protein Using Mn ²⁺ Tags. Journal of Physical Chemistry Letters, 2012, 3, 157-160.	4.6	72
27	Determining the Oligomeric Structure of Proteorhodopsin by Gd ³⁺ -Based Pulsed Dipolar Spectroscopy of Multiple Distances. Structure, 2014, 22, 1677-1686.	3.3	72
28	An Inflammatory Role for the Mammalian Carboxypeptidase Inhibitor Latexin: Relationship to Cystatins and the Tumor Suppressor TIG1. Structure, 2005, 13, 309-317.	3.3	71
29	Structural basis for recruitment of tandem hotdog domains in acyl-CoA thioesterase 7 and its role in inflammation. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 10382-10387.	7.1	71
30	Predicting disulfide connectivity from protein sequence using multiple sequence feature vectors and secondary structure. Bioinformatics, 2007, 23, 3147-3154.	4.1	65
31	Translational incorporation of L-3,4-dihydroxyphenylalanine into proteins. FEBS Journal, 2005, 272, 3162-3171.	4.7	64
32	SWARM-MD: Searching Conformational Space by Cooperative Molecular Dynamics. Journal of Physical Chemistry A, 1998, 102, 5937-5943.	2.5	63
33	Protein contact prediction using patterns of correlation. Proteins: Structure, Function and Bioinformatics, 2004, 56, 679-684.	2.6	63
34	Predikin and PredikinDB: a computational framework for the prediction of protein kinase peptide specificity and an associated database of phosphorylation sites. BMC Bioinformatics, 2008, 9, 245.	2.6	62
35	Crystallography and proteinâ€™protein interactions: biological interfaces and crystal contacts. Biochemical Society Transactions, 2008, 36, 1438-1441.	3.4	61
36	Sequence-Specific and Stereospecific Assignment of Methyl Groups Using Paramagnetic Lanthanides. Journal of the American Chemical Society, 2007, 129, 13749-13757.	13.7	59

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37	Efficient $\tilde{\chi}$ -tensor determination and NH assignment of paramagnetic proteins. <i>Journal of Biomolecular NMR</i> , 2006, 35, 79-87.	2.8	56
38	Gadolinium(III) Spin Labels for High-Sensitivity Distance Measurements in Transmembrane Helices. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 11831-11834.	13.8	54
39	Sensitive NMR Approach for Determining the Binding Mode of Tightly Binding Ligand Molecules to Protein Targets. <i>Journal of the American Chemical Society</i> , 2016, 138, 4539-4546.	13.7	53
40	W-band orientation selective DEER measurements on a Gd ³⁺ /nitroxide mixed-labeled protein dimer with a dual mode cavity. <i>Journal of Magnetic Resonance</i> , 2013, 227, 66-71.	2.1	52
41	Terahertz and far infrared Spectroscopy of alanine-rich peptides having variable ellipticity. <i>Optics Express</i> , 2010, 18, 27431.	3.4	51
42	3-Mercapto-2,6-Pyridinedicarboxylic Acid: A Small Lanthanide-Binding Tag for Protein Studies by NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2010, 16, 3827-3832.	3.3	50
43	The structure of the PII-ATP complex. <i>FEBS Journal</i> , 2001, 268, 2028-2037.	0.2	48
44	Biocompatible Macrocyclization between Cysteine and 2-Cyanopyridine Generates Stable Peptide Inhibitors. <i>Organic Letters</i> , 2019, 21, 4709-4712.	4.6	46
45	Engineering of a bis-chelator motif into a protein α -helix for rigid lanthanide binding and paramagnetic NMR spectroscopy. <i>Chemical Communications</i> , 2011, 47, 7368.	4.1	44
46	Phosphoregulators: Protein Kinases and Protein Phosphatases of Mouse. <i>Genome Research</i> , 2003, 13, 1443-1454.	5.5	43
47	Magic Angle Spinning NMR Structure Determination of Proteins from Pseudocontact Shifts. <i>Journal of the American Chemical Society</i> , 2013, 135, 8294-8303.	13.7	42
48	Flexibility of NS5 Methyltransferase-Polymerase Linker Region Is Essential for Dengue Virus Replication. <i>Journal of Virology</i> , 2015, 89, 10717-10721.	3.4	41
49	Wurst: a protein threading server with a structural scoring function, sequence profiles and optimized substitution matrices. <i>Nucleic Acids Research</i> , 2004, 32, W532-W535.	14.5	40
50	Structure Optimization Combining Soft-Core Interaction Functions, the Diffusion Equation Method, and Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5926-5930.	2.5	36
51	Intramolecular binding mode of the C-terminus of <i>Escherichia coli</i> single-stranded DNA binding protein determined by nuclear magnetic resonance spectroscopy. <i>Nucleic Acids Research</i> , 2014, 42, 2750-2757.	14.5	36
52	Proofreading exonuclease on a tether: the complex between the E. coli DNA polymerase III subunits $\hat{\alpha}$, $\hat{\mu}$, $\hat{\gamma}$, and $\hat{\delta}$ reveals a highly flexible arrangement of the proofreading domain. <i>Nucleic Acids Research</i> , 2013, 41, 5354-5367.	14.5	34
53	Generation of Pseudocontact Shifts in Protein NMR Spectra with a Genetically Encoded Cobalt(II)-Binding Amino Acid. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 692-694.	13.8	33
54	Site-Specific Incorporation of Selenocysteine by Genetic Encoding as a Photocaged Unnatural Amino Acid. <i>Bioconjugate Chemistry</i> , 2018, 29, 2257-2264.	3.6	33

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55	Paramagpy: software for fitting magnetic susceptibility tensors using paramagnetic effects measured in NMR spectra. <i>Magnetic Resonance</i> , 2020, 1, 1-12.	1.9	33
56	uPEPperoni: An online tool for upstream open reading frame location and analysis of transcript conservation. <i>BMC Bioinformatics</i> , 2014, 15, 36.	2.6	32
57	Cortactin Adopts a Globular Conformation and Bundles Actin into Sheets. <i>Journal of Biological Chemistry</i> , 2008, 283, 16187-16193.	3.4	29
58	Capturing Conformational States in Proteins Using Sparse Paramagnetic NMR Data. <i>PLoS ONE</i> , 2015, 10, e0127053.	2.5	29
59	Coupling constants again: Experimental restraints in structure refinement. <i>Journal of Computer-Aided Molecular Design</i> , 1994, 8, 29-40.	2.9	28
60	Structure of the N-Terminal Domain of Escherichia coli Glutamine Synthetase Adenylyltransferase. <i>Structure</i> , 2004, 12, 861-869.	3.3	28
61	4,4'-Dithiobisdipicolinic Acid: A Small and Convenient Lanthanide Binding Tag for Protein NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2011, 17, 6830-6836.	3.3	28
62	<i>tert</i> -Butyltyrosine, an NMR Tag for High-Molecular-Weight Systems and Measurements of Submicromolar Ligand Binding Affinities. <i>Journal of the American Chemical Society</i> , 2015, 137, 4581-4586.	13.7	28
63	Characterization of Low-Frequency Modes in Aqueous Peptides Using Far-Infrared Spectroscopy and Molecular Dynamics Simulation. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11559-11565.	2.5	27
64	Engineering [Ln(DPA) ₃] ³⁺ binding sites in proteins: a widely applicable method for tagging proteins with lanthanide ions. <i>Journal of Biomolecular NMR</i> , 2011, 50, 411-420.	2.8	26
65	Pseudocontact Shift-Driven Iterative Resampling for 3D Structure Determinations of Large Proteins. <i>Journal of Molecular Biology</i> , 2016, 428, 522-532.	4.2	26
66	Double-Arm Lanthanide Tags Deliver Narrow Gd ³⁺ Distance Distributions in Double Electron Resonance (DEER) Measurements. <i>Chemistry - A European Journal</i> , 2017, 23, 11694-11702.	3.3	25
67	Protein fold recognition without Boltzmann statistics or explicit physical basis. <i>Protein Science</i> , 1998, 7, 142-149.	7.6	24
68	Identification of Disulfide-Containing Chemical Cross-Links in Proteins Using MALDI-TOF/TOF-Mass Spectrometry. <i>Analytical Chemistry</i> , 2008, 80, 5036-5043.	6.5	24
69	Far-infrared spectroscopy analysis of linear and cyclic peptides, and lysozyme. <i>Vibrational Spectroscopy</i> , 2012, 61, 144-150.	2.2	24
70	Tunable paramagnetic relaxation enhancements by [Gd(DPA) ₃] ³⁺ for protein structure analysis. <i>Journal of Biomolecular NMR</i> , 2010, 47, 143-153.	2.8	23
71	Probing the solution structure of the E. coli multidrug transporter MdfA using DEER distance measurements with nitroxide and Gd(III) spin labels. <i>Scientific Reports</i> , 2019, 9, 12528.	3.3	23
72	Directed Evolution of New and Improved Enzyme Functions Using an Evolutionary Intermediate and Multidirectional Search. <i>ACS Chemical Biology</i> , 2015, 10, 611-621.	3.4	22

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73	Genetic Encoding of <i>para</i> -Pentafluorosulfanyl Phenylalanine: A Highly Hydrophobic and Strongly Electronegative Group for Stable Protein Interactions. <i>Journal of the American Chemical Society</i> , 2020, 142, 17277-17281.	13.7	22
74	Structural Proteomics. <i>Methods in Molecular Biology</i> , 2008, 426, v-vi.	0.9	21
75	Modelling the structure of latexin-carboxypeptidase A complex based on chemical cross-linking and molecular docking. <i>Protein Engineering, Design and Selection</i> , 2006, 19, 9-16.	2.1	19
76	Genetic Encoding of <i>N</i> ⁶ -(((Trimethylsilyl)methoxy)carbonyl)-lysine for NMR Studies of Protein-Protein and Protein-Ligand Interactions. <i>Journal of the American Chemical Society</i> , 2021, 143, 1133-1143.	13.7	18
77	Protein Structure Determination Using a Combination of Cross-linking, Mass Spectrometry, and Molecular Modeling. <i>Methods in Molecular Biology</i> , 2008, 426, 459-474.	0.9	18
78	Analysis of the solution conformations of T4 lysozyme by paramagnetic NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5850-5859.	2.8	17
79	Protein Structure Determination by Assembling Super-Secondary Structure Motifs Using Pseudocontact Shifts. <i>Structure</i> , 2017, 25, 559-568.	3.3	17
80	Through-Space Scalar ¹⁹ F- ¹⁹ F Couplings between Fluorinated Noncanonical Amino Acids for the Detection of Specific Contacts in Proteins. <i>Journal of the American Chemical Society</i> , 2021, 143, 19587-19598.	13.7	16
81	Sausage: protein threading with flexible force fields. <i>Bioinformatics</i> , 1999, 15, 1064-1065.	4.1	15
82	Site-selective tagging of proteins by pnictogen-mediated self-assembly. <i>Chemical Communications</i> , 2017, 53, 10894-10897.	4.1	15
83	Genetic Encoding of Cyanopyridylalanine for In-Cell Protein Macrocyclization by the Nitrile-Amino Thiol Click Reaction. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	15
84	Optimization methods for conformational sampling using a Boltzmann-weighted mean field approach. <i>Biopolymers</i> , 1998, 39, 103-114.	2.4	14
85	Focusing in on structural genomics: The University of Queensland structural biology pipeline. <i>New Biotechnology</i> , 2006, 23, 281-289.	2.7	14
86	Identification of a non-purple tartrate-resistant acid phosphatase: an evolutionary link to Ser/Thr protein phosphatases?. <i>BMC Research Notes</i> , 2008, 1, 78.	1.4	13
87	Site-specific tagging proteins with a rigid, small and stable transition metal chelator, 8-hydroxyquinoline, for paramagnetic NMR analysis. <i>Journal of Biomolecular NMR</i> , 2016, 64, 103-113.	2.8	13
88	Two Histidines in an Î±-Helix: A Rigid Co ²⁺ -Binding Motif for PCS Measurements by NMR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 6226-6229.	13.8	12
89	Molecular dynamics simulation using weak-coupling NOE distance restraining. <i>Journal of Biomolecular NMR</i> , 1996, 8, 285-291.	2.8	11
90	Protein sequence threading, the alignment problem, and a two-step strategy. <i>Journal of Computational Chemistry</i> , 1999, 20, 1455-1467.	3.3	10

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91	Three-Dimensional Protein Structure Determination Using Pseudocontact Shifts of Backbone Amide Protons Generated by Double-Histidine Co ²⁺ -Binding Motifs at Multiple Sites. <i>Biochemistry</i> , 2019, 58, 3243-3250.	2.5	10
92	Site-Specific Incorporation of 7-Fluoro-L-tryptophan into Proteins by Genetic Encoding to Monitor Ligand Binding by ¹⁹ F NMR Spectroscopy. <i>ACS Sensors</i> , 2022, 7, 44-49.	7.8	9
93	<i>In Vitro</i> Protein Synthesis in Semipermeable Artificial Cells. <i>ACS Synthetic Biology</i> , 2021, 10, 1237-1244.	3.8	8
94	Computational chemistry on Fujitsu vectorâ€“parallel processors: Development and performance of applications software. <i>Parallel Computing</i> , 2000, 26, 887-911.	2.1	7
95	Pilot studies on the parallel production of soluble mouse proteins in a bacterial expression system. <i>Journal of Structural and Functional Genomics</i> , 2005, 6, 13-20.	1.2	7
96	An Introduction to Protein Contact Prediction. <i>Methods in Molecular Biology</i> , 2008, 453, 87-104.	0.9	7
97	3D Computational Modeling of Proteins Using Sparse Paramagnetic NMR Data. <i>Methods in Molecular Biology</i> , 2017, 1526, 3-21.	0.9	6
98	Optimization methods for conformational sampling using a Boltzmannâ€“weighted mean field approach. <i>Biopolymers</i> , 1996, 39, 103-114.	2.4	6
99	Modern Biocatalysis. <i>RSC Catalysis Series</i> , 2018, , .	0.1	5
100	Protein fold recognition score functions: Unusual construction strategies. , 1999, 36, 454-461.		4
101	Transformation of hemipentahydrate to monohydrate of risedronate monosodium by seed crystallization in solution. <i>AIChE Journal</i> , 2011, 57, 3385-3394.	3.6	4
102	Cellâ€“Free Synthesis of Selenoproteins in High Yield and Purity for Selective Protein Tagging. <i>ChemBioChem</i> , 2021, 22, 1480-1486.	2.6	4
103	Comment on 'Protein isoelectric point as a predictor for increased crystallization screening efficiency'. <i>Bioinformatics</i> , 2004, 20, 2169-2170.	4.1	3
104	Free energy approximations in simple lattice proteins. <i>Journal of Chemical Physics</i> , 2001, 114, 4998-5005.	3.0	2
105	A General Target Selection Method for Crystallographic Proteomics. <i>Methods in Molecular Biology</i> , 2008, 426, 27-35.	0.9	2
106	PGASâ€“FMM: Implementing a distributed fast multipole method using the X10 programming language. <i>Concurrency Computation Practice and Experience</i> , 2014, 26, 712-727.	2.2	2
107	Two Histidines in an Î±-Helix: A Rigid Co ²⁺ -Binding Motif for PCS Measurements by NMR Spectroscopy. <i>Angewandte Chemie</i> , 2018, 130, 6334-6337.	2.0	2
108	Overview of the Pipeline for Structural and Functional Characterization of Macrophage Proteins at the University of Queensland. <i>Methods in Molecular Biology</i> , 2008, 426, 577-587.	0.9	1

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109	Organoarsenic probes to study proteins by NMR spectroscopy. Chemical Communications, 2022, 58, 701-704.	4.1	1
110	2P001 1F1450 A cell-free system for highly efficient incorporation of unnatural amino acids for studies of protein-protein interactions(The 48th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2010, 50, S82.	0.1	0
111	Genetic Encoding of Cyanopyridylalanine for Inâ€Cell Protein Macrocyclization by the Nitrileâ€Aminothiol Click Reaction. Angewandte Chemie, 0, , .	2.0	0