Thomas Huber

List of Publications by Year
in descending order

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111 papers	18,204 citations	57631 44 h-index	24179 110 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.	1.4	9,859
2	Bellerophon: a program to detect chimeric sequences in multiple sequence alignments. Bioinformatics, 2004, 20, 2317-2319.	1.8	1,443
3	The GROMOS Biomolecular Simulation Program Package. Journal of Physical Chemistry A, 1999, 103, 3596-3607.	1.1	1,354
4	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	9.0	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.	1.3	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.	0.8	203
7	Numbat: an interactive software tool for fitting Î”Ï‡-tensors to molecular coordinates using pseudocontact shifts. Journal of Biomolecular NMR, 2008, 41, 179-189.	1.6	168
8	Nanometer-Scale Distance Measurements in Proteins Using Gd³⁺ Spin Labeling. Journal of the American Chemical Society, 2010, 132, 9040-9048.	6.6	143
9	Structure refinement using time-averaged J-coupling constant restraints. Journal of Biomolecular NMR, 1993, 3, 55-66.	1.6	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.	6.6	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.	6.6	117
12	Protein Structure Determination from Pseudocontact Shifts Using ROSETTA. Journal of Molecular Biology, 2012, 416, 668-677.	2.0	106
13	DOTA-Amide Lanthanide Tag for Reliable Generation of Pseudocontact Shifts in Protein NMR Spectra. Bioconjugate Chemistry, 2011, 22, 2118-2125.	1.8	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.	6.6	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.	6.6	96
16	3D structure determination of a protein in living cells using paramagnetic NMR spectroscopy. Chemical Communications, 2016, 52, 10237-10240.	2.2	90
17	Systematic Characterization of the Zinc-Finger-Containing Proteins in the Mouse Transcriptome. Genome Research, 2003, 13, 1430-1442.	2.4	89
18	Multipleâ€Site Labeling of Proteins with Unnatural Amino Acids. Angewandte Chemie - International Edition, 2012, 51, 2243-2246.	7.2	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.	3.5	85
20	Fast Structure-Based Assignment of15N HSQC Spectra of Selectively15N-Labeled Paramagnetic Proteins. Journal of the American Chemical Society, 2004, 126, 2963-2970.	6.6	83
21	Prediction of cis/trans isomerization in proteins using PSI-BLAST profiles and secondary structure information. BMC Bioinformatics, 2006, 7, 124.	1.2	83
22	Site-Specific Labelling of Proteins with a Rigid Lanthanide-Binding Tag. ChemBioChem, 2006, 7, 1599-1604.	1.3	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.	1.8	81
24	Three-Dimensional Protein Fold Determination from Backbone Amide Pseudocontact Shifts Generated by Lanthanide Tags at Multiple Sites. Structure, 2013, 21, 883-890.	1.6	77
25	Spectroscopic selection of distance measurements in a protein dimer with mixed nitroxide and Gd3+ spin labels. Physical Chemistry Chemical Physics, 2012, 14, 4355.	1.3	73
26	Nanometer-Range Distance Measurement in a Protein Using Mn²⁺ Tags. Journal of Physical Chemistry Letters, 2012, 3, 157-160.	2.1	72
27	Determining the Oligomeric Structure of Proteorhodopsin by Gd3+-Based Pulsed Dipolar Spectroscopy of Multiple Distances. Structure, 2014, 22, 1677-1686.	1.6	72
28	An Inflammatory Role for the Mammalian Carboxypeptidase Inhibitor Latexin: Relationship to Cystatins and the Tumor Suppressor TIG1. Structure, 2005, 13, 309-317.	1.6	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.	3.3	71
30	Predicting disulfide connectivity from protein sequence using multiple sequence feature vectors and secondary structure. Bioinformatics, 2007, 23, 3147-3154.	1.8	65
31	Translational incorporation of L-3,4-dihydroxyphenylalanine into proteins. FEBS Journal, 2005, 272, 3162-3171.	2.2	64
32	SWARM-MD:Â Searching Conformational Space by Cooperative Molecular Dynamics. Journal of Physical Chemistry A, 1998, 102, 5937-5943.	1.1	63
33	Protein contact prediction using patterns of correlation. Proteins: Structure, Function and Bioinformatics, 2004, 56, 679-684.	1.5	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.	1.2	62
35	Crystallography and proteinâ€“protein interactions: biological interfaces and crystal contacts. Biochemical Society Transactions, 2008, 36, 1438-1441.	1.6	61
36	Sequence-Specific and Stereospecific Assignment of Methyl Groups Using Paramagnetic Lanthanides. Journal of the American Chemical Society, 2007, 129, 13749-13757.	6.6	59

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37	Efficient Ï‡-tensor determination and NH assignment of paramagnetic proteins. Journal of Biomolecular NMR, 2006, 35, 79-87.	1.6	56
38	Gadolinium(III) Spin Labels for Highâ€Sensitivity Distance Measurements in Transmembrane Helices. Angewandte Chemie - International Edition, 2013, 52, 11831-11834.	7.2	54
39	Sensitive NMR Approach for Determining the Binding Mode of Tightly Binding Ligand Molecules to Protein Targets. Journal of the American Chemical Society, 2016, 138, 4539-4546.	6.6	53
40	W-band orientation selective DEER measurements on a Gd3+/nitroxide mixed-labeled protein dimer with a dual mode cavity. Journal of Magnetic Resonance, 2013, 227, 66-71.	1.2	52
41	Terahertz and far infrared Spectroscopy of alanine-rich peptides having variable ellipticity. Optics Express, 2010, 18, 27431.	1.7	51
42	3â€Mercaptoâ€2,6â€Pyridinedicarboxylic Acid: A Small Lanthanideâ€Binding Tag for Protein Studies by NMR Spectroscopy. Chemistry - A European Journal, 2010, 16, 3827-3832.	1.7	50
43	The structure of the PII-ATP complex. FEBS Journal, 2001, 268, 2028-2037.	0.2	48
44	Biocompatible Macrocyclization between Cysteine and 2-Cyanopyridine Generates Stable Peptide Inhibitors. Organic Letters, 2019, 21, 4709-4712.	2.4	46
45	Engineering of a bis-chelator motif into a protein Î±-helix for rigid lanthanide binding and paramagnetic NMR spectroscopy. Chemical Communications, 2011, 47, 7368.	2.2	44
46	Phosphoregulators: Protein Kinases and Protein Phosphatases of Mouse. Genome Research, 2003, 13, 1443-1454.	2.4	43
47	Magic Angle Spinning NMR Structure Determination of Proteins from Pseudocontact Shifts. Journal of the American Chemical Society, 2013, 135, 8294-8303.	6.6	42
48	Flexibility of NS5 Methyltransferase-Polymerase Linker Region Is Essential for Dengue Virus Replication. Journal of Virology, 2015, 89, 10717-10721.	1.5	41
49	Wurst: a protein threading server with a structural scoring function, sequence profiles and optimized substitution matrices. Nucleic Acids Research, 2004, 32, W532-W535.	6.5	40
50	Structure Optimization Combining Soft-Core Interaction Functions, the Diffusion Equation Method, and Molecular Dynamics. Journal of Physical Chemistry A, 1997, 101, 5926-5930.	1.1	36
51	Intramolecular binding mode of the C-terminus ofEscherichia colisingle-stranded DNA binding protein determined by nuclear magnetic resonance spectroscopy. Nucleic Acids Research, 2014, 42, 2750-2757.	6.5	36
52	Proofreading exonuclease on a tether: the complex between the E. coli DNA polymerase III subunits Î±, Îµ, Î¸ and Î² reveals a highly flexible arrangement of the proofreading domain. Nucleic Acids Research, 2013, 41, 5354-5367.	6.5	34
53	Generation of Pseudocontact Shifts in Protein NMR Spectra with a Genetically Encoded Cobalt(II)â€Binding Amino Acid. Angewandte Chemie - International Edition, 2011, 50, 692-694.	7.2	33
54	Site-Specific Incorporation of Selenocysteine by Genetic Encoding as a Photocaged Unnatural Amino Acid. Bioconjugate Chemistry, 2018, 29, 2257-2264.	1.8	33

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55	Paramagpy: software for fitting magnetic susceptibility tensors using paramagnetic effects measured in NMR spectra. Magnetic Resonance, 2020, 1, 1-12.	0.8	33
56	uPEPperoni: An online tool for upstream open reading frame location and analysis of transcript conservation. BMC Bioinformatics, 2014, 15, 36.	1.2	32
57	Cortactin Adopts a Globular Conformation and Bundles Actin into Sheets. Journal of Biological Chemistry, 2008, 283, 16187-16193.	1.6	29
58	Capturing Conformational States in Proteins Using Sparse Paramagnetic NMR Data. PLoS ONE, 2015, 10, e0127053.	1.1	29
59	Coupling constants again: Experimental restraints in structure refinement. Journal of Computer-Aided Molecular Design, 1994, 8, 29-40.	1.3	28
60	Structure of the N-Terminal Domain of Escherichia coli Glutamine Synthetase Adenylyltransferase. Structure, 2004, 12, 861-869.	1.6	28
61	4,4â€²â€Dithiobisdipicolinic Acid: A Small and Convenient Lanthanide Binding Tag for Protein NMR Spectroscopy. Chemistry - A European Journal, 2011, 17, 6830-6836.	1.7	28
62	O-tert-Butyltyrosine, an NMR Tag for High-Molecular-Weight Systems and Measurements of Submicromolar Ligand Binding Affinities. Journal of the American Chemical Society, 2015, 137, 4581-4586.	6.6	28
63	Characterization of Low-Frequency Modes in Aqueous Peptides Using Far-Infrared Spectroscopy and Molecular Dynamics Simulation. Journal of Physical Chemistry A, 2011, 115, 11559-11565.	1.1	27
64	Engineering [Ln(DPA)3]3â^' binding sites in proteins: a widely applicable method for tagging proteins with lanthanide ions. Journal of Biomolecular NMR, 2011, 50, 411-420.	1.6	26
65	Pseudocontact Shift-Driven Iterative Resampling for 3D Structure Determinations of Large Proteins. Journal of Molecular Biology, 2016, 428, 522-532.	2.0	26
66	Doubleâ€Arm Lanthanide Tags Deliver Narrow Gd³⁺â€“Gd³⁺ Distance Distributions in Double Electronâ€“Electron Resonance (DEER) Measurements. Chemistry - A European Journal, 2017, 23, 11694-11702.	1.7	25
67	Protein fold recognition without Boltzmann statistics or explicit physical basis. Protein Science, 1998, 7, 142-149.	3.1	24
68	Identification of Disulfide-Containing Chemical Cross-Links in Proteins Using MALDI-TOF/TOF-Mass Spectrometry. Analytical Chemistry, 2008, 80, 5036-5043.	3.2	24
69	Far-infrared spectroscopy analysis of linear and cyclic peptides, and lysozyme. Vibrational Spectroscopy, 2012, 61, 144-150.	1.2	24
70	Tunable paramagnetic relaxation enhancements by [Gd(DPA)3]3â^' for protein structure analysis. Journal of Biomolecular NMR, 2010, 47, 143-153.	1.6	23
71	Probing the solution structure of the E. coli multidrug transporter MdfA using DEER distance measurements with nitroxide and Gd(III) spin labels. Scientific Reports, 2019, 9, 12528.	1.6	23
72	Directed Evolution of New and Improved Enzyme Functions Using an Evolutionary Intermediate and Multidirectional Search. ACS Chemical Biology, 2015, 10, 611-621.	1.6	22

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73	Genetic Encoding of para-Pentafluorosulfanyl Phenylalanine: A Highly Hydrophobic and Strongly Electronegative Group for Stable Protein Interactions. Journal of the American Chemical Society, 2020, 142, 17277-17281.	6.6	22
74	Structural Proteomics. Methods in Molecular Biology, 2008, 426, v-vi.	0.4	21
75	Modelling the structure of latexinâ€“carboxypeptidase A complex based on chemical cross-linking and molecular docking. Protein Engineering, Design and Selection, 2006, 19, 9-16.	1.0	19
76	Genetic Encoding of N⁶-(((Trimethylsilyl)methoxy)carbonyl)-<scp>l</scp>-lysine for NMR Studies of Proteinâ€“Protein and Proteinâ€“Ligand Interactions. Journal of the American Chemical Society, 2021, 143, 1133-1143.	6.6	18
77	Protein Structure Determination Using a Combination of Cross-linking, Mass Spectrometry, and Molecular Modeling. Methods in Molecular Biology, 2008, 426, 459-474.	0.4	18
78	Analysis of the solution conformations of T4 lysozyme by paramagnetic NMR spectroscopy. Physical Chemistry Chemical Physics, 2016, 18, 5850-5859.	1.3	17
79	Protein Structure Determination by Assembling Super-Secondary Structure Motifs Using Pseudocontact Shifts. Structure, 2017, 25, 559-568.	1.6	17
80	Through-Space Scalar ¹⁹Fâ€“¹⁹F Couplings between Fluorinated Noncanonical Amino Acids for the Detection of Specific Contacts in Proteins. Journal of the American Chemical Society, 2021, 143, 19587-19598.	6.6	16
81	Sausage: protein threading with flexible force fields. Bioinformatics, 1999, 15, 1064-1065.	1.8	15
82	Site-selective tagging of proteins by pnictogen-mediated self-assembly. Chemical Communications, 2017, 53, 10894-10897.	2.2	15
83	Genetic Encoding of Cyanopyridylalanine for Inâ€Cell Protein Macrocyclization by the Nitrileâ€“Aminothiol Click Reaction. Angewandte Chemie - International Edition, 2022, 61, .	7.2	15
84	Optimization methods for conformational sampling using a Boltzmann-weighted mean field approach. Biopolymers, 1998, 39, 103-114.	1.2	14
85	Focusing in on structural genomics: The University of Queensland structural biology pipeline. New Biotechnology, 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?. BMC Research Notes, 2008, 1, 78.	0.6	13
87	Site-specific tagging proteins with a rigid, small and stable transition metal chelator, 8-hydroxyquinoline, for paramagnetic NMR analysis. Journal of Biomolecular NMR, 2016, 64, 103-113.	1.6	13
88	Two Histidines in an Î±â€Helix: A Rigid Co²⁺â€Binding Motif for PCS Measurements by NMR Spectroscopy. Angewandte Chemie - International Edition, 2018, 57, 6226-6229.	7.2	12
89	Molecular dynamics simulation using weak-coupling NOE distance restraining. Journal of Biomolecular NMR, 1996, 8, 285-291.	1.6	11
90	Protein sequence threading, the alignment problem, and a two-step strategy. Journal of Computational Chemistry, 1999, 20, 1455-1467.	1.5	10

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91	Three-Dimensional Protein Structure Determination Using Pseudocontact Shifts of Backbone Amide Protons Generated by Double-Histidine Co²⁺-Binding Motifs at Multiple Sites. Biochemistry, 2019, 58, 3243-3250.	1.2	10
92	Site-Specific Incorporation of 7-Fluoro-<scp>L</scp>-tryptophan into Proteins by Genetic Encoding to Monitor Ligand Binding by ¹⁹F NMR Spectroscopy. ACS Sensors, 2022, 7, 44-49.	4.0	9
93	In Vitro Protein Synthesis in Semipermeable Artificial Cells. ACS Synthetic Biology, 2021, 10, 1237-1244.	1.9	8
94	Computational chemistry on Fujitsu vectorâ€“parallel processors: Development and performance of applications software. Parallel Computing, 2000, 26, 887-911.	1.3	7
95	Pilot studies on the parallel production of soluble mouse proteins in a bacterial expression system. Journal of Structural and Functional Genomics, 2005, 6, 13-20.	1.2	7
96	An Introduction to Protein Contact Prediction. Methods in Molecular Biology, 2008, 453, 87-104.	0.4	7
97	3D Computational Modeling of Proteins Using Sparse Paramagnetic NMR Data. Methods in Molecular Biology, 2017, 1526, 3-21.	0.4	6
98	Optimization methods for conformational sampling using a Boltzmann-weighted mean field approach. , 1996, 39, 103.		6
99	Modern Biocatalysis. RSC Catalysis Series, 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. AICHE Journal, 2011, 57, 3385-3394.	1.8	4
102	Cellâ€Free Synthesis of Selenoproteins in High Yield and Purity for Selective Protein Tagging. ChemBioChem, 2021, 22, 1480-1486.	1.3	4
103	Comment on 'Protein isoelectric point as a predictor for increased crystallization screening efficiency'. Bioinformatics, 2004, 20, 2169-2170.	1.8	3
104	Free energy approximations in simple lattice proteins. Journal of Chemical Physics, 2001, 114, 4998-5005.	1.2	2
105	A General Target Selection Method for Crystallographic Proteomics. Methods in Molecular Biology, 2008, 426, 27-35.	0.4	2
106	PGASâ€FMM: Implementing a distributed fast multipole method using the X10 programming language. Concurrency Computation Practice and Experience, 2014, 26, 712-727.	1.4	2
107	Two Histidines in an Î±â€Helix: A Rigid Co²⁺â€Binding Motif for PCS Measurements by NMR Spectroscopy. Angewandte Chemie, 2018, 130, 6334-6337.	1.6	2
108	Overview of the Pipeline for Structural and Functional Characterization of Macrophage Proteins at the University of Queensland. Methods in Molecular Biology, 2008, 426, 577-587.	0.4	1

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109	Organoarsenic probes to study proteins by NMR spectroscopy. Chemical Communications, 2022, 58, 701-704.	2.2	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.	0.0	0
111	Genetic Encoding of Cyanopyridylalanine for Inâ€Cell Protein Macrocyclization by the Nitrileâ€Aminothiol Click Reaction. Angewandte Chemie, 0, , .	1.6	0