

# Thomas Szyperski

## List of Publications by Year in descending order

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95  
papers

6,719  
citations

94433

37  
h-index

62596

80  
g-index

132  
all docs

132  
docs citations

132  
times ranked

6098  
citing authors

#	ARTICLE	IF	CITATIONS
1	From Protein Design to the Energy Landscape of a Cold Unfolding Protein. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1212-1231.	2.6	3
2	Oligomeric interactions maintain active-site structure in a noncooperative enzyme family. <i>EMBO Journal</i> , 2022, 41, .	7.8	10
3	Perturbing the energy landscape for improved packing during computational protein design. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 436-449.	2.6	85
4	Hanudatta S. Atreya (1974–2020). <i>Magnetic Resonance in Chemistry</i> , 2021, 59, 201-212.	1.9	0
5	Evolutionary coupling saturation mutagenesis: Coevolution-guided identification of distant sites influencing <i>Bacillus naganensis</i> pullulanase activity. <i>FEBS Letters</i> , 2020, 594, 799-812.	2.8	22
6	Folding and Assembly of Short $\alpha$ , $\beta$ , $\beta$ -Hybrid Peptides: Minor Variations in Sequence and Drastic Differences in Higher-Level Structures. <i>Journal of the American Chemical Society</i> , 2019, 141, 14239-14248.	13.7	18
7	Structural Basis by Which the N-Terminal Polypeptide Segment of <i>Rhizopus chinensis</i> Lipase Regulates Its Substrate Binding Affinity. <i>Biochemistry</i> , 2019, 58, 3943-3954.	2.5	14
8	Development of a Fragment-Based Screening Assay for the Focal Adhesion Targeting Domain Using SPR and NMR. <i>Molecules</i> , 2019, 24, 3352.	3.8	10
9	The copBL operon protects <i>Staphylococcus aureus</i> from copper toxicity: CopL is an extracellular membrane-associated copper-binding protein. <i>Journal of Biological Chemistry</i> , 2019, 294, 4027-4044.	3.4	34
10	Cytosolic expression, solution structures, and molecular dynamics simulation of genetically encodable disulfide-rich <i>de novo</i> designed peptides. <i>Protein Science</i> , 2018, 27, 1611-1623.	7.6	14
11	Room Temperature X-Ray Crystallography Reveals Conformational Heterogeneity of Engineered Proteins. <i>Structure</i> , 2017, 25, 691-692.	3.3	2
12	<sup>13</sup> C metabolic flux profiling of <i>Pichia pastoris</i> grown in aerobic batch cultures on glucose revealed high relative anabolic use of TCA cycle and limited incorporation of provided precursors of branched-chain amino acids. <i>FEBS Journal</i> , 2017, 284, 3100-3113.	4.7	10
13	Aromatic oligureas as hosts for anions and cations. <i>Chemical Communications</i> , 2016, 52, 9905-9908.	4.1	10
14	A community resource of experimental data for NMR / X-ray crystal structure pairs. <i>Protein Science</i> , 2016, 25, 30-45.	7.6	24
15	Accurate <i>de novo</i> design of hyperstable constrained peptides. <i>Nature</i> , 2016, 538, 329-335.	27.8	327
16	Metabolomics of biomarker discovery in ovarian cancer: a systematic review of the current literature. <i>Metabolomics</i> , 2016, 12, 1.	3.0	57
17	Discrete Stacking of Aromatic Oligoamide Macrocycles. <i>Journal of the American Chemical Society</i> , 2015, 137, 5879-5882.	13.7	37
18	Solution NMR Experiment for Measurement of <sup>15</sup> N- <sup>1</sup> H Residual Dipolar Couplings in Large Proteins and Supramolecular Complexes. <i>Journal of the American Chemical Society</i> , 2015, 137, 11242-11245.	13.7	10

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19	Polypeptide backbone, C <sup>1</sup> and methyl group resonance assignments of the 24 kDa plectin repeat domain 6 from human protein plectin. <i>Biomolecular NMR Assignments</i> , 2015, 9, 135-138.	0.8	0
20	High-Quality NMR Structure of Human Anti-Apoptotic Protein Domain Mcl-1(171-327) for Cancer Drug Design. <i>PLoS ONE</i> , 2014, 9, e96521.	2.5	24
21	Structural and Functional Characterization of DUF1471 Domains of Salmonella Proteins SrfN, YdgH/SssB, and YahO. <i>PLoS ONE</i> , 2014, 9, e101787.	2.5	13
22	Spatially Selective Heteronuclear Multiple-Quantum Coherence Spectroscopy for Biomolecular NMR Studies. <i>ChemPhysChem</i> , 2014, 15, 1872-1879.	2.1	6
23	Identification of Low-Molecular-Weight Compounds Inhibiting Growth of Corynebacteria: Potential Lead Compounds for Antibiotics. <i>ChemMedChem</i> , 2014, 9, 282-285.	3.2	3
24	Solution NMR structures of homeodomains from human proteins ALX4, ZHX1, and CASP8AP2 contribute to the structural coverage of the Human Cancer Protein Interaction Network. <i>Journal of Structural and Functional Genomics</i> , 2014, 15, 201-207.	1.2	1
25	Solution NMR structures of immunoglobulin-like domains 7 and 12 from obscurin-like protein 1 contribute to the structural coverage of the human cancer protein interaction network. <i>Journal of Structural and Functional Genomics</i> , 2014, 15, 209-214.	1.2	0
26	Solution NMR structure of the helicase associated domain BVU_0683(627-691) from <i>Bacteroides vulgatus</i> provides first structural coverage for protein domain family PF03457 and indicates domain binding to DNA. <i>Journal of Structural and Functional Genomics</i> , 2013, 14, 19-24.	1.2	0
27	Solution NMR structure of CD1104B from pathogenic <i>Clostridium difficile</i> reveals a distinct $\alpha$ -helical architecture and provides first structural representative of protein domain family PF14203. <i>Journal of Structural and Functional Genomics</i> , 2013, 14, 155-160.	1.2	2
28	Protein Conformational Space Populated in Solution Probed with Aromatic Residual Dipolar Couplings. <i>ChemBioChem</i> , 2013, 14, 684-688.	2.6	14
29	Solution NMR structures provide first structural coverage of the large protein domain family PF08369 and complementary structural coverage of dark operative protochlorophyllide oxidoreductase complexes. <i>Journal of Structural and Functional Genomics</i> , 2013, 14, 119-126.	1.2	0
30	<sup>1</sup> H NMR based profiling of spent culture media cannot predict success of implantation for day 3 human embryos. <i>Journal of Assisted Reproduction and Genetics</i> , 2012, 29, 1435-1442.	2.5	17
31	GFT projection NMR for efficient <sup>1</sup> H/ <sup>13</sup> C sugar spin system identification in nucleic acids. <i>Journal of Biomolecular NMR</i> , 2012, 54, 337-342.	2.8	4
32	Highly Precise Measurement of Kinetic Isotope Effects Using <sup>1</sup> H-Detected 2D [ <sup>13</sup> C, <sup>1</sup> H]-HSQC NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2012, 134, 20589-20592.	13.7	33
33	Solution NMR structures reveal unique homodimer formation by a winged helix-turn-helix motif and provide first structures for protein domain family PF10771. <i>Journal of Structural and Functional Genomics</i> , 2012, 13, 1-7.	1.2	2
34	Solution NMR structures reveal a distinct architecture and provide first structures for protein domain family PF04536. <i>Journal of Structural and Functional Genomics</i> , 2012, 13, 9-14.	1.2	7
35	Increasing Sequence Diversity with Flexible Backbone Protein Design: The Complete Redesign of a Protein Hydrophobic Core. <i>Structure</i> , 2012, 20, 1086-1096.	3.3	58
36	NMR Structure of Lipoprotein YxeF from <i>Bacillus subtilis</i> Reveals a Calycin Fold and Distant Homology with the Lipocalin Blc from <i>Escherichia coli</i> . <i>PLoS ONE</i> , 2012, 7, e37404.	2.5	6

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37	Diagnosis of Early Stage Ovarian Cancer by <sup>1</sup> H NMR Metabonomics of Serum Explored by Use of a Microflow NMR Probe. <i>Journal of Proteome Research</i> , 2011, 10, 1765-1771.	3.7	70
38	Theory of mirrored time domain sampling for NMR spectroscopy. <i>Journal of Magnetic Resonance</i> , 2011, 213, 46-57.	2.1	2
39	NMR-based structural biology of proteins in supercooled water. <i>Journal of Structural and Functional Genomics</i> , 2011, 12, 1-7.	1.2	14
40	Solution NMR structure of MED25(391â€“543) comprising the activator-interacting domain (ACID) of human mediator subunit 25. <i>Journal of Structural and Functional Genomics</i> , 2011, 12, 159-166.	1.2	18
41	Solution NMR structures of proteins VPA0419 from <i>Vibrio parahaemolyticus</i> and yiiS from <i>Shigella flexneri</i> provide structural coverage for protein domain family PFAM 04175. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 779-784.	2.6	0
42	NMR Structure Determination for Larger Proteins Using Backbone-Only Data. <i>Science</i> , 2010, 327, 1014-1018.	12.6	245
43	Advances in protein NMR provided by the NIGMS Protein Structure Initiative: impact on drug discovery. <i>Current Opinion in Drug Discovery &amp; Development</i> , 2010, 13, 335-49.	1.9	7
44	Analysis of the Varicella-Zoster Virus IE62 N-Terminal Acidic Transactivating Domain and Its Interaction with the Human Mediator Complex. <i>Journal of Virology</i> , 2009, 83, 6300-6305.	3.4	26
45	Standard operating procedure for metabonomics studies of blood serum and plasma samples using a <sup>1</sup> H NMR microflow probe. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, S81-5.	1.9	15
46	Clean Absorption Mode NMR Data Acquisition. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 1479-1483.	13.8	6
47	Unique opportunities for NMR methods in structural genomics. <i>Journal of Structural and Functional Genomics</i> , 2009, 10, 101-106.	1.2	25
48	Clean absorption mode NMR data acquisition based on time-proportional phase incrementation. <i>Journal of Structural and Functional Genomics</i> , 2009, 10, 227-232.	1.2	5
49	Structure of the Protein BPTI Derived with NOESY in Supercooled Water: Validation and Refinement of Solution Structures. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 324-326.	13.8	5
50	Consistent blind protein structure generation from NMR chemical shift data. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 4685-4690.	7.1	776
51	Simultaneously Cycled NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2008, 130, 4925-4933.	13.7	8
52	On NMR-based Structural Proteomics. , 2008, , 307-329.		0
53	J-GFT NMR for Precise Measurement of Mutually Correlated Nuclear Spin-Spin Couplings. <i>Journal of the American Chemical Society</i> , 2007, 129, 680-692.	13.7	24
54	Metabolic flux profiling of <i>Pichia pastoris</i> grown on glycerol/methanol mixtures in chemostat cultures at low and high dilution rates. <i>Microbiology (United Kingdom)</i> , 2007, 153, 281-290.	1.8	82

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55	Combined NMR-observation of cold denaturation in supercooled water and heat denaturation enables accurate measurement of $^1\text{H}$ p of protein unfolding. <i>European Biophysics Journal</i> , 2006, 35, 363-366.	2.2	43
56	Principles and applications of GFT projection NMR spectroscopy. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, S51-S60.	1.9	51
57	NMR solution structure of <i>Thermotoga maritima</i> protein TM1509 reveals a Zn-metalloprotease-like tertiary structure. <i>Journal of Structural and Functional Genomics</i> , 2005, 6, 51-62.	1.2	21
58	An Integrated Platform for Automated Analysis of Protein NMR Structures. <i>Methods in Enzymology</i> , 2005, 394, 111-141.	1.0	67
59	Rapid NMR Data Collection. <i>Methods in Enzymology</i> , 2005, 394, 78-108.	1.0	86
60	NMR data collection and analysis protocol for high-throughput protein structure determination. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 10487-10492.	7.1	108
61	Probing Structure and Functional Dynamics of (Large) Proteins with Aromatic Rings: $\hat{\text{A}}$ L-GFT-TROSY (4,3)DHCCH NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2005, 127, 14578-14579.	13.7	32
62	G-Matrix Fourier Transform NOESY-Based Protocol for High-Quality Protein Structure Determination. <i>Journal of the American Chemical Society</i> , 2005, 127, 9085-9099.	13.7	54
63	Resonance Assignment of Proteins with High Shift Degeneracy Based on 5D Spectral Information Encoded in G2FT NMR Experiments. <i>Journal of the American Chemical Society</i> , 2005, 127, 4554-4555.	13.7	35
64	Amino acid biosynthesis and metabolic flux profiling of <i>Pichia pastoris</i> . <i>FEBS Journal</i> , 2004, 271, 2462-2470.	0.2	82
65	GFT NMR Experiments for Polypeptide Backbone and $^{13}\text{C}$ Chemical Shift Assignment. <i>Journal of Biomolecular NMR</i> , 2004, 28, 117-130.	2.8	38
66	A generalized approach to automated NMR peak list editing: application to reduced dimensionality triple resonance spectra. <i>Journal of Magnetic Resonance</i> , 2004, 170, 263-277.	2.1	38
67	The phosphoenolpyruvate carboxykinase also catalyzes C3 carboxylation at the interface of glycolysis and the TCA cycle of <i>Bacillus subtilis</i> . <i>Metabolic Engineering</i> , 2004, 6, 277-284.	7.0	49
68	G-matrix Fourier transform NMR spectroscopy for complete protein resonance assignment. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 9642-9647.	7.1	125
69	GFT NMR, a New Approach To Rapidly Obtain Precise High-Dimensional NMR Spectral Information. <i>Journal of the American Chemical Society</i> , 2003, 125, 1385-1393.	13.7	340
70	Metabolic-Flux Profiling of the Yeasts <i>Saccharomyces cerevisiae</i> and <i>Pichia stipitis</i> . <i>Eukaryotic Cell</i> , 2003, 2, 170-180.	3.4	150
71	Reduced-dimensionality NMR spectroscopy for high-throughput protein resonance assignment. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 8009-8014.	7.1	186
72	Metabolic Flux Responses to Pyruvate Kinase Knockout in <i>Escherichia coli</i> . <i>Journal of Bacteriology</i> , 2002, 184, 152-164.	2.2	254

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73	Strukturelle Genomik. Nachrichten Aus Der Chemie, 2002, 50, 1128-1131.	0.0	3
74	Intracellular Carbon Fluxes in Riboflavin-Producing <i>Bacillus subtilis</i> during Growth on Two-Carbon Substrate Mixtures. Applied and Environmental Microbiology, 2002, 68, 1760-1771.	3.1	70
75	Protein dynamics in supercooled water: the search for slow motional modes. Journal of Biomolecular NMR, 2002, 23, 63-67.	2.8	32
76	Central carbon metabolism of <i>Saccharomyces cerevisiae</i> explored by biosynthetic fractional <sup>13</sup> C labeling of common amino acids. FEBS Journal, 2001, 268, 2464-2479.	0.2	151
77	Aromatic Ring-Flipping in Supercooled Water: Implications for NMR-Based Structural Biology of Proteins. Journal of the American Chemical Society, 2001, 123, 388-397.	13.7	72
78	Metabolic flux response to phosphoglucose isomerase knock-out in <i>Escherichia coli</i> and impact of overexpression of the soluble transhydrogenase UdhA. FEMS Microbiology Letters, 2001, 204, 247-252.	1.8	160
79	Dissection of Central Carbon Metabolism of Hemoglobin-Expressing <i>Escherichia coli</i> by <sup>13</sup> C Nuclear Magnetic Resonance Flux Distribution Analysis in Microaerobic Bioprocesses. Applied and Environmental Microbiology, 2001, 67, 680-687.	3.1	35
80	Metabolic flux response to phosphoglucose isomerase knock-out in <i>Escherichia coli</i> and impact of overexpression of the soluble transhydrogenase UdhA. FEMS Microbiology Letters, 2001, 204, 247-252.	1.8	9
81	Toward Structural Biology in Supercooled Water. Journal of the American Chemical Society, 2000, 122, 3230-3231.	13.7	43
82	Metabolic Flux Ratio Analysis of Genetic and Environmental Modulations of <i>Escherichia coli</i> Central Carbon Metabolism. Journal of Bacteriology, 1999, 181, 6679-6688.	2.2	361
83	Bioreaction Network Topology and Metabolic Flux Ratio Analysis by Biosynthetic Fractional <sup>13</sup> C Labeling and Two-Dimensional NMR Spectroscopy. Metabolic Engineering, 1999, 1, 189-197.	7.0	103
84	The 2D <sup>31</sup> P Spin-Echo-Difference Constant-Time [ <sup>13</sup> C, <sup>1</sup> H]-HMQC Experiment for Simultaneous Determination of <sup>3</sup> J <sub>H3â€²P and <sup>3</sup>J<sub>C4â€²P in <sup>13</sup>C-Labeled Nucleic Acids and Their Protein Complexes. Journal of Magnetic Resonance, 1999, 140, 491-494.</sub></sub>	2.1	20
85	Conformational Changes of the BS2 Operator DNA upon Complex Formation with the Antennapedia Homeodomain Studied by NMR with <sup>13</sup> C/ <sup>15</sup> N-labeled DNA. Journal of Molecular Biology, 1999, 292, 609-617.	4.2	14
86	Amino Acid Biosynthesis in the Halophilic Archaeon <i>Haloarcula hispanica</i> . Journal of Bacteriology, 1999, 181, 3226-3237.	2.2	45
87	Title is missing!. Journal of Biomolecular NMR, 1998, 11, 387-405.	2.8	36
88	Measurement of Deoxyribose <sup>3</sup> J <sub>HHS</sub> Scalar Couplings Reveals Protein Binding-Induced Changes in the Sugar Puckers of the DNA. Journal of the American Chemical Society, 1998, 120, 821-822.	13.7	18
89	<sup>13</sup> C-NMR, MS and metabolic flux balancing in biotechnology research. Quarterly Reviews of Biophysics, 1998, 31, 41-106.	5.7	216
90	Measurement of <sup>3</sup> J <sub>C2â€²P</sub> Scalar Couplings in a 17 kDa Protein Complex with <sup>13</sup> C, <sup>15</sup> N-Labeled DNA Distinguishes the Bland BII Phosphate Conformations of the DNA. Journal of the American Chemical Society, 1997, 119, 9901-9902.	13.7	33

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91	Metabolic fluxes in riboflavin-producing <i>Bacillus subtilis</i> . <i>Nature Biotechnology</i> , 1997, 15, 448-452.	17.5	241
92	Detecting and dissecting metabolic fluxes using biosynthetic fractional <sup>13</sup> C labeling and two-dimensional NMR spectroscopy. <i>Trends in Biotechnology</i> , 1996, 14, 453-459.	9.3	60
93	Biosynthetically Directed Fractional <sup>13</sup> C-labeling of Proteinogenic Amino Acids. An Efficient Analytical Tool to Investigate Intermediary Metabolism. <i>FEBS Journal</i> , 1995, 232, 433-448.	0.2	335
94	Support of <sup>1</sup> H NMR assignments in proteins by biosynthetically directed fractional <sup>13</sup> C-labeling. <i>Journal of Biomolecular NMR</i> , 1992, 2, 323-334.	2.8	99
95	Stereospecific nuclear magnetic resonance assignments of the methyl groups of valine and leucine in the DNA-binding domain of the 434 repressor by biosynthetically directed fractional carbon- <sup>13</sup> labeling. <i>Biochemistry</i> , 1989, 28, 7510-7516.	2.5	597