Thomas Szyperski

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

93 5,861 35 76 g-index

132 6,340 8.5 ext. papers ext. citations avg, IF L-index

#	Paper	IF	Citations
93	Perturbing the energy landscape for improved packing during computational protein design. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021 , 89, 436-449	4.2	22
92	Evolutionary coupling saturation mutagenesis: Coevolution-guided identification of distant sites influencing Bacillus naganoensis pullulanase activity. <i>FEBS Letters</i> , 2020 , 594, 799-812	3.8	10
91	Structural Basis by Which the N-Terminal Polypeptide Segment of Lipase Regulates Its Substrate Binding Affinity. <i>Biochemistry</i> , 2019 , 58, 3943-3954	3.2	9
90	Development of a Fragment-Based Screening Assay for the Focal Adhesion Targeting Domain Using SPR and NMR. <i>Molecules</i> , 2019 , 24,	4.8	8
89	Folding and Assembly of Short IDEHybrid Peptides: Minor Variations in Sequence and Drastic Differences in Higher-Level Structures. <i>Journal of the American Chemical Society</i> , 2019 , 141, 14239-1424	18 ^{6.4}	10
88	The operon protects from copper toxicity: CopL is an extracellular membrane-associated copper-binding protein. <i>Journal of Biological Chemistry</i> , 2019 , 294, 4027-4044	5.4	23
87	Cytosolic expression, solution structures, and molecular dynamics simulation of genetically encodable disulfide-rich de novo designed peptides. <i>Protein Science</i> , 2018 , 27, 1611-1623	6.3	11
86	Room Temperature X-Ray Crystallography Reveals Conformational Heterogeneity of Engineered Proteins. <i>Structure</i> , 2017 , 25, 691-692	5.2	1
85	C metabolic flux profiling of Pichia pastoris 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	5.7	8
84	Accurate de novo design of hyperstable constrained peptides. <i>Nature</i> , 2016 , 538, 329-335	50.4	231
83	Metabolomics of biomarker discovery in ovarian cancer: a systematic review of the current literature. <i>Metabolomics</i> , 2016 , 12, 1	4.7	42
82	Aromatic oligureas as hosts for anions and cations. <i>Chemical Communications</i> , 2016 , 52, 9905-8	5.8	9
81	A community resource of experimental data for NMR / X-ray crystal structure pairs. <i>Protein Science</i> , 2016 , 25, 30-45	6.3	10
80	Discrete stacking of aromatic oligoamide macrocycles. <i>Journal of the American Chemical Society</i> , 2015 , 137, 5879-82	16.4	27
79	Solution NMR Experiment for Measurement of (15)N-(1)H Residual Dipolar Couplings in Large Proteins and Supramolecular Complexes. <i>Journal of the American Chemical Society</i> , 2015 , 137, 11242-5	16.4	7
78	Polypeptide backbone, C(Dand 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	0.7	
77	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, 201-7		1

(2011-2014)

Solution NMR structures of immunoglobulin-like domains 7 and 12 from obscurin-like protein 1 76 contribute to the structural coverage of the Human Cancer Protein Interaction Network. Journal of Structural and Functional Genomics, 2014, 15, 209-14 High-quality NMR structure of human anti-apoptotic protein domain Mcl-1(171-327) for cancer 20 75 3.7 drug design. PLoS ONE, 2014, 9, e96521 Structural and functional characterization of DUF1471 domains of Salmonella proteins SrfN, 8 74 3.7 YdgH/SssB, and YahO. *PLoS ONE*, **2014**, 9, e101787 Spatially selective heteronuclear multiple-quantum coherence spectroscopy for biomolecular NMR 6 3.2 studies. ChemPhysChem, 2014, 15, 1872-9 Identification of low-molecular-weight compounds inhibiting growth of corynebacteria: potential 72 3.7 3 lead compounds for antibiotics. ChemMedChem, 2014, 9, 282-5 Solution NMR structure of the helicase associated domain BVU 0683(627-691) from Bacteroides vulgatus provides first structural coverage for protein domain family PF03457 and indicates 71 domain binding to DNA. Journal of Structural and Functional Genomics, 2013, 14, 19-24 Solution NMR structure of CD1104B from pathogenic Clostridium difficile reveals a distinct Ehelical architecture and provides first structural representative of protein domain family 70 1 PF14203. Journal of Structural and Functional Genomics, 2013, 14, 155-60 Protein conformational space populated in solution probed with aromatic residual dipolar (13) C-(1) 3.8 69 12 H couplings. *ChemBioChem*, **2013**, 14, 684-8 Solution NMR structures provide first structural coverage of the large protein domain family PF08369 and complementary structural coverage of dark operative protochlorophyllide 68 oxidoreductase complexes. Journal of Structural and Functional Genomics, 2013, 14, 119-26 Increasing sequence diversity with flexible backbone protein design: the complete redesign of a 67 5.2 45 protein hydrophobic core. Structure, 2012, 20, 1086-96 (1)H NMR based profiling of spent culture media cannot predict success of implantation for day 3 66 14 3.4 human embryos. Journal of Assisted Reproduction and Genetics, 2012, 29, 1435-42 GFT projection NMR for efficient (1)H/ (13)C sugar spin system identification in nucleic acids. 65 4 Journal of Biomolecular NMR, 2012, 54, 337-42 Highly precise measurement of kinetic isotope effects using 1H-detected 2D [13C,1H]-HSQC NMR 64 16.4 32 spectroscopy. Journal of the American Chemical Society, 2012, 134, 20589-92 Solution NMR structures reveal unique homodimer formation by a winged helix-turn-helix motif and provide first structures for protein domain family PF10771. Journal of Structural and Functional 63 2 *Genomics*, **2012**, 13, 1-7 Solution NMR structures reveal a distinct architecture and provide first structures for protein 62 7 domain family PF04536. Journal of Structural and Functional Genomics, 2012, 13, 9-14 NMR structure of lipoprotein YxeF from Bacillus subtilis reveals a calycin fold and distant homology 61 3.7 with the lipocalin Blc from Escherichia coli. PLoS ONE, 2012, 7, e37404 Theory of mirrored time domain sampling for NMR spectroscopy. Journal of Magnetic Resonance, 60 3 2 **2011**, 213, 46-57 NMR-based structural biology of proteins in supercooled water. Journal of Structural and Functional 59 13 Genomics, **2011**, 12, 1-7

58	Solution NMR structure of MED25(391-543) comprising the activator-interacting domain (ACID) of human mediator subunit 25. <i>Journal of Structural and Functional Genomics</i> , 2011 , 12, 159-66		13
57	Diagnosis of early stage ovarian cancer by 1H NMR metabonomics of serum explored by use of a microflow NMR probe. <i>Journal of Proteome Research</i> , 2011 , 10, 1765-71	5.6	58
56	NMR structure determination for larger proteins using backbone-only data. <i>Science</i> , 2010 , 327, 1014-8	33.3	220
55	Solution NMR structures of proteins VPA0419 from Vibrio parahaemolyticus and yiiS from Shigella flexneri provide structural coverage for protein domain family PFAM 04175. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 779-84	4.2	
54	Advances in protein NMR provided by the NIGMS Protein Structure Initiative: impact on drug discovery. <i>Current Opinion in Drug Discovery & Development</i> , 2010 , 13, 335-49		7
53	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, 6300-5	6.6	23
52	Clean Absorption-Mode NMR Data Acquisition. <i>Angewandte Chemie</i> , 2009 , 121, 1507-1511	3.6	2
51	Standard operating procedure for metabonomics studies of blood serum and plasma samples using a 1H-NMR micro-flow probe. <i>Magnetic Resonance in Chemistry</i> , 2009 , 47 Suppl 1, S81-5	2.1	13
50	Clean absorption-mode NMR data acquisition. Angewandte Chemie - International Edition, 2009, 48, 147	918634	4
49	Unique opportunities for NMR methods in structural genomics. <i>Journal of Structural and Functional Genomics</i> , 2009 , 10, 101-6		15
48	Clean absorption mode NMR data acquisition based on time-proportional phase incrementation. Journal of Structural and Functional Genomics, 2009 , 10, 227-32		4
47	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, 4685-90	11.5	665
46	Simultaneously cycled NMR spectroscopy. <i>Journal of the American Chemical Society</i> , 2008 , 130, 4925-33	16.4	8
45	On NMR-based Structural Proteomics 2008 , 307-329		
44	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, 324-6	16.4	5
43	J-GFT NMR for precise measurement of mutually correlated nuclear spin-spin couplings. <i>Journal of the American Chemical Society</i> , 2007 , 129, 680-92	16.4	24
42	Metabolic flux profiling of Pichia pastoris grown on glycerol/methanol mixtures in chemostat cultures at low and high dilution rates. <i>Microbiology (United Kingdom)</i> , 2007 , 153, 281-90	2.9	74
41	Combined NMR-observation of cold denaturation in supercooled water and heat denaturation enables accurate measurement of deltaC(p) of protein unfolding. European Biophysics Journal, 2006	1.9	35

(2002-2006)

40	Principles and applications of GFT projection NMR spectroscopy. <i>Magnetic Resonance in Chemistry</i> , 2006 , 44 Spec No, S51-60	2.1	46	
39	Probing structure and functional dynamics of (large) proteins with aromatic rings: L-GFT-TROSY (4,3)D HCCH NMR spectroscopy. <i>Journal of the American Chemical Society</i> , 2005 , 127, 14578-9	16.4	31	
38	G-matrix Fourier transform NOESY-based protocol for high-quality protein structure determination. Journal of the American Chemical Society, 2005 , 127, 9085-99	16.4	54	
37	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, 4554-5	16.4	34	
36	NMR solution structure of Thermotoga maritima protein TM1509 reveals a Zn-metalloprotease-like tertiary structure. <i>Journal of Structural and Functional Genomics</i> , 2005 , 6, 51-62		19	
35	An integrated platform for automated analysis of protein NMR structures. <i>Methods in Enzymology</i> , 2005 , 394, 111-41	1.7	59	
34	Rapid NMR data collection. <i>Methods in Enzymology</i> , 2005 , 394, 78-108	1.7	78	
33	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, 10487-92	11.5	101	
32	Amino acid biosynthesis and metabolic flux profiling of Pichia pastoris. FEBS Journal, 2004, 271, 2462-	70	74	
31	GFT NMR experiments for polypeptide backbone and 13Cbeta chemical shift assignment. <i>Journal of Biomolecular NMR</i> , 2004 , 28, 117-30	3	37	
30	A generalized approach to automated NMR peak list editing: application to reduced dimensionality triple resonance spectra. <i>Journal of Magnetic Resonance</i> , 2004 , 170, 263-77	3	36	
29	The phosphoenolpyruvate carboxykinase also catalyzes C3 carboxylation at the interface of glycolysis and the TCA cycle of Bacillus subtilis. <i>Metabolic Engineering</i> , 2004 , 6, 277-84	9.7	45	
28	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, 9642-7	11.5	118	
27	GFT NMR, a new approach to rapidly obtain precise high-dimensional NMR spectral information. <i>Journal of the American Chemical Society</i> , 2003 , 125, 1385-93	16.4	322	
26	Metabolic-flux profiling of the yeasts Saccharomyces cerevisiae and Pichia stipitis. <i>Eukaryotic Cell</i> , 2003 , 2, 170-80		133	
25	Protein dynamics in supercooled water: the search for slow motional modes. <i>Journal of Biomolecular NMR</i> , 2002 , 23, 63-7	3	30	
24	Reduced-dimensionality NMR spectroscopy for high-throughput protein resonance assignment.	11.5	165	
	Proceedings of the National Academy of Sciences of the United States of America, 2002 , 99, 8009-14			

22	Strukturelle Genomik. <i>Nachrichten Aus Der Chemie</i> , 2002 , 50, 1128-1131	0.1	3
21	Intracellular carbon fluxes in riboflavin-producing Bacillus subtilis during growth on two-carbon substrate mixtures. <i>Applied and Environmental Microbiology</i> , 2002 , 68, 1760-71	4.8	64
20	Central carbon metabolism of Saccharomyces cerevisiae explored by biosynthetic fractional (13)C labeling of common amino acids. <i>FEBS Journal</i> , 2001 , 268, 2464-79		133
19	Aromatic ring-flipping in supercooled water: implications for NMR-based structural biology of proteins. <i>Journal of the American Chemical Society</i> , 2001 , 123, 388-97	16.4	65
18	Metabolic flux response to phosphoglucose isomerase knock-out in Escherichia coli and impact of overexpression of the soluble transhydrogenase UdhA. <i>FEMS Microbiology Letters</i> , 2001 , 204, 247-52	2.9	147
17	Dissection of central carbon metabolism of hemoglobin-expressing Escherichia coli by 13C nuclear magnetic resonance flux distribution analysis in microaerobic bioprocesses. <i>Applied and Environmental Microbiology</i> , 2001 , 67, 680-7	4.8	33
16	Toward Structural Biology in Supercooled Water. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3230-3231	16.4	41
15	Metabolic flux ratio analysis of genetic and environmental modulations of Escherichia coli central carbon metabolism. <i>Journal of Bacteriology</i> , 1999 , 181, 6679-88	3.5	323
14	Bioreaction network topology and metabolic flux ratio analysis by biosynthetic fractional 13C labeling and two-dimensional NMR spectroscopy. <i>Metabolic Engineering</i> , 1999 , 1, 189-97	9.7	96
13	The 2D [31P] spin-echo-difference constant-time [13C, 1H]-HMQC experiment for simultaneous determination of 3J(H3P) and 3J(C4P) in 13C-labeled nucleic acids and their protein complexes. <i>Journal of Magnetic Resonance</i> , 1999 , 140, 491-4	3	18
12	Conformational changes of the BS2 operator DNA upon complex formation with the Antennapedia homeodomain studied by NMR with 13C/15N-labeled DNA. <i>Journal of Molecular Biology</i> , 1999 , 292, 609	-97	11
11	Amino acid biosynthesis in the halophilic archaeon Haloarcula hispanica. <i>Journal of Bacteriology</i> , 1999 , 181, 3226-37	3.5	36
10	Sequential resonance assignment of medium-sized15 N/13C-labeled proteins with projected 4D triple resonance NMR experiments. <i>Journal of Biomolecular NMR</i> , 1998 , 11, 387-405	3	25
9	Measurement of Deoxyribose 3JHH Scalar Couplings Reveals Protein Binding-Induced Changes in the Sugar Puckers of the DNA. <i>Journal of the American Chemical Society</i> , 1998 , 120, 821-822	16.4	16
8	13C-NMR, MS and metabolic flux balancing in biotechnology research. <i>Quarterly Reviews of Biophysics</i> , 1998 , 31, 41-106	7	194
7	Measurement of 3JC2 B Scalar Couplings in a 17 kDa Protein Complex with 13C,15N-Labeled DNA Distinguishes the BI and BII Phosphate Conformations of the DNA. <i>Journal of the American Chemical Society</i> , 1997 , 119, 9901-9902	16.4	30
6	Metabolic fluxes in riboflavin-producing Bacillus subtilis. <i>Nature Biotechnology</i> , 1997 , 15, 448-52	44.5	221
5	Detecting and dissecting metabolic fluxes using biosynthetic fractional 13C labeling and two-dimensional NMR spectroscopy. <i>Trends in Biotechnology</i> , 1996 , 14, 453-459	15.1	58

LIST OF PUBLICATIONS

4	Biosynthetically directed fractional 13C-labeling of proteinogenic amino acids. An efficient analytical tool to investigate intermediary metabolism. <i>FEBS Journal</i> , 1995 , 232, 433-48		305
3	Support of 1H NMR assignments in proteins by biosynthetically directed fractional 13C-labeling. Journal of Biomolecular NMR, 1992 , 2, 323-34	3	88
2	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 13C labeling. <i>Biochemistry</i> , 1989 , 28, 7510-6	3.2	564
1	Metabolic flux response to phosphoglucose isomerase knock-out in Escherichia coli and impact of overexpression of the soluble transhydrogenase UdhA		8