Wolfram Gronwald

List of Publications by Year
in descending order

70 papers	2,870 citations	186265 28 h-index	175258 52 g-index
71 all docs	71 docs citations	71 times ranked	4984 citing authors

#	ARTICLE	IF	CITATIONS
1	Combined chemical shift changes and amino acid specific chemical shift mapping of protein–protein interactions. Journal of Biomolecular NMR, 2007, 39, 275-289.	2.8	200
2	State-of-the art data normalization methods improve NMR-based metabolomic analysis. Metabolomics, 2012, 8, 146-160.	3.0	196
3	Advances in amino acid analysis. Analytical and Bioanalytical Chemistry, 2009, 393, 445-452.	3.7	168
4	A Metabolome-Wide Association Study of Kidney Function and Disease in the General Population. Journal of the American Society of Nephrology: JASN, 2016, 27, 1175-1188.	6.1	159
5	Automated GC–MS analysis of free amino acids in biological fluids. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2008, 870, 222-232.	2.3	158
6	Urinary Metabolite Quantification Employing 2D NMR Spectroscopy. Analytical Chemistry, 2008, 80, 9288-9297.	6.5	123
7	NMR Metabolomic Analysis of Dairy Cows Reveals Milk Glycerophosphocholine to Phosphocholine Ratio as Prognostic Biomarker for Risk of Ketosis. Journal of Proteome Research, 2012, 11, 1373-1381.	3.7	122
8	Unusual β-sheet periodicity in small cyclic peptides. Nature Structural Biology, 1998, 5, 284-288.	9.7	111
9	Automated structure determination of proteins by NMR spectroscopy. Progress in Nuclear Magnetic Resonance Spectroscopy, 2004, 44, 33-96.	7.5	98
10	Solution NMR structure of the cold-shock protein from the hyperthermophilic bacterium Thermotoga maritima. FEBS Journal, 2001, 268, 2527-2539.	0.2	97
11	New Aspects of an Old Drug – Diclofenac Targets MYC and Glucose Metabolism in Tumor Cells. PLoS ONE, 2013, 8, e66987.	2.5	86
12	Diclofenac inhibits lactate formation and efficiently counteracts local immune suppression in a murine glioma model. International Journal of Cancer, 2013, 132, 843-853.	5.1	77
13	Detection of autosomal dominant polycystic kidney disease by NMR spectroscopic fingerprinting of urine. Kidney International, 2011, 79, 1244-1253.	5.2	59
14	Automated assignment of NOESY NMR spectra using a knowledge based method (KNOWNOE). Journal of Biomolecular NMR, 2002, 23, 271-287.	2.8	53
15	Mitochondrial DNA copy number is associated with mortality and infections in a large cohort of patients with chronic kidney disease. Kidney International, 2019, 96, 480-488.	5.2	53
16	Solution Structure of the Ras Binding Domain of the Protein Kinase Byr2 from Schizosaccharomyces pombe. Structure, 2001, 9, 1029-1041.	3.3	52
17	RFAC, a program for automated NMR R-factor estimation. Journal of Biomolecular NMR, 2000, 17, 137-151.	2.8	50
18	CAMRA: chemical shift based computer aided protein NMR assignments. Journal of Biomolecular NMR, 1998, 12, 395-405.	2.8	46

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19	Infrequent cavity-forming fluctuations in HPr from Staphylococcus carnosus revealed by pressure- and temperature-dependent tyrosine ring flips. Protein Science, 2009, 13, 3104-3114.	7.6	45
20	Comparison of serum versus plasma collection in gas chromatography – Mass spectrometry–based metabolomics. Electrophoresis, 2010, 31, 2365-2373.	2.4	43
21	Genome-Wide Association Studies of Metabolites in Patients with CKD Identify Multiple Loci and Illuminate Tubular Transport Mechanisms. Journal of the American Society of Nephrology: JASN, 2018, 29, 1513-1524.	6.1	39
22	Structure of the Leech Protein Saratin and Characterization of Its Binding to Collagen. Journal of Molecular Biology, 2008, 381, 913-927.	4.2	36
23	Performance Evaluation of Algorithms for the Classification of Metabolic ^{1}H NMR Fingerprints. Journal of Proteome Research, 2012, 11, 6242-6251.	3.7	33
24	Data Normalization of ^{1}H NMR Metabolite Fingerprinting Data Sets in the Presence of Unbalanced Metabolite Regulation. Journal of Proteome Research, 2015, 14, 3217-3228.	3.7	32
25	Statistical Analysis of NMR Metabolic Fingerprints: Established Methods and Recent Advances. Metabolites, 2018, 8, 47.	2.9	32
26	Residual Dipolar Couplings in Short Peptidic Foldamers: Combined Analyses of Backbone and Side–Chain Conformations and Evaluation of Structure Coordinates of Rigid Unnatural Amino Acids. ChemBioChem, 2009, 10, 440-444.	2.6	30
27	Discrimination of steatosis and NASH in mice using nuclear magnetic resonance spectroscopy. Metabolomics, 2011, 7, 237-246.	3.0	30
28	Structure Determination and Ligand Interactions of the PDZ2b Domain of PTP-Bas (hPTP1E): Splicing-induced Modulation of Ligand Specificity. Journal of Molecular Biology, 2003, 334, 143-155.	4.2	29
29	Distinct metabolic differences between various human cancer and primary cells. Electrophoresis, 2013, 34, 2836-2847.	2.4	29
30	Analysis of human urine reveals metabolic changes related to the development of acute kidney injury following cardiac surgery. Metabolomics, 2013, 9, 697-707.	3.0	28
31	Early changes in the liver–soluble proteome from mice fed a nonalcoholic steatohepatitis inducing diet. Proteomics, 2012, 12, 1437-1451.	2.2	26
32	Visceral adipose tissue but not subcutaneous adipose tissue is associated with urine and serum metabolites. PLoS ONE, 2017, 12, e0175133.	2.5	26
33	Systematic Evaluation of Non-Uniform Sampling Parameters in the Targeted Analysis of Urine Metabolites by 1H,1H 2D NMR Spectroscopy. Scientific Reports, 2018, 8, 4249.	3.3	26
34	High CD206 levels in Hodgkin lymphoma–educated macrophages are linked to matrix–remodeling and lymphoma dissemination. Molecular Oncology, 2020, 14, 571-589.	4.6	25
35	Correlations between Milk and Plasma Levels of Amino and Carboxylic Acids in Dairy Cows. Journal of Proteome Research, 2013, 12, 5223-5232.	3.7	24
36	Quantification of Metabolites by NMR Spectroscopy in the Presence of Protein. Journal of Proteome Research, 2017, 16, 1784-1796.	3.7	24

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37	Targeting Melanoma Metastasis and Immunosuppression with a New Mode of Melanoma Inhibitory Activity (MIA) Protein Inhibition. PLoS ONE, 2012, 7, e37941.	2.5	23
38	PROCOS: Computational analysis of protein–protein complexes. Journal of Computational Chemistry, 2011, 32, 2575-2586.	3.3	22
39	Polymorphisms within the *APOBR* gene are highly associated with milk levels of prognostic ketosis biomarkers in dairy cows. Physiological Genomics, 2015, 47, 129-137.	2.3	22
40	Comprehensive Metaboproteomics of Burkitt's and Diffuse Large B-Cell Lymphoma Cell Lines and Primary Tumor Tissues Reveals Distinct Differences in Pyruvate Content and Metabolism. Journal of Proteome Research, 2017, 16, 1105-1120.	3.7	22
41	Evaluation of dilution and normalization strategies to correct for urinary output in HPLC-HRTOFMS metabolomics. Analytical and Bioanalytical Chemistry, 2016, 408, 8483-8493.	3.7	21
42	A Predictive Model for Progression of CKD to Kidney Failure Based on Routine Laboratory Tests. American Journal of Kidney Diseases, 2022, 79, 217-230.e1.	1.9	21
43	External calibration with *Drosophila* whole-cell spike-ins delivers absolute mRNA fold changes from human RNA-Seq and qPCR data. BioTechniques, 2017, 62, 53-61.	1.8	20
44	MetaboQuant: a tool combining individual peak calibration and outlier detection for accurate metabolite quantification in 1D ^{1}H and ^{1}H-^{13}C HSQC NMR spectra. BioTechniques, 2013, 54, 251-256.	1.8	19
45	ORB, a homology-based program for the prediction of protein NMR chemical shifts. Journal of Biomolecular NMR, 1997, 10, 165-179.	2.8	18
46	Identification of Plasma Metabolites Prognostic of Acute Kidney Injury after Cardiac Surgery with Cardiopulmonary Bypass. Journal of Proteome Research, 2015, 14, 2897-2905.	3.7	18
47	Non-Invasive Prediction of IDH Mutation in Patients with Glioma WHO II/III/IV Based on F-18-FET PET-Guided In Vivo 1H-Magnetic Resonance Spectroscopy and Machine Learning. Cancers, 2020, 12, 3406.	3.7	17
48	Current Experimental, Bioinformatic and Statistical Methods used in NMR Based Metabolomics. Current Metabolomics, 2013, 1, 253-268.	0.5	16
49	Results from the German Chronic Kidney Disease (GCKD) study support association of relative telomere length with mortality in a large cohort of patients with moderate chronic kidney disease. Kidney International, 2020, 98, 488-497.	5.2	16
50	Scale-Invariant Biomarker Discovery in Urine and Plasma Metabolite Fingerprints. Journal of Proteome Research, 2017, 16, 3596-3605.	3.7	15
51	A multi-source data integration approach reveals novel associations between metabolites and renal outcomes in the German Chronic Kidney Disease study. Scientific Reports, 2019, 9, 13954.	3.3	15
52	A Novel Metabolic Signature To Predict the Requirement of Dialysis or Renal Transplantation in Patients with Chronic Kidney Disease. Journal of Proteome Research, 2019, 18, 1796-1805.	3.7	15
53	Assessment by 1H NMR Spectroscopy of the Structural Behaviour of Human Parathyroid-Hormone-Related Protein(1 - 34) and Its Close Relationship with the N-Terminal Fragments of Human Parathyroid Hormone in Solution. Biological Chemistry, 1997, 378, 1501-8.	2.5	13
54	Improved simulation of NOESY spectra by RELAX-JT2 including effects of J-coupling, transverse relaxation and chemical shift anisotropy. Journal of Biomolecular NMR, 2004, 30, 121-131.	2.8	12

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55	AUREMOL-RFAC-3D, combination of R-factors and their use for automated quality assessment of protein solution structures. Journal of Biomolecular NMR, 2006, 37, 15-30.	2.8	11
56	An R-Package for the Deconvolution and Integration of 1D NMR Data: MetaboDecon1D. Metabolites, 2021, 11, 452.	2.9	9
57	Cytokine-specific autoantibodies shape the gut microbiome in autoimmune polyendocrine syndrome type 1. Journal of Allergy and Clinical Immunology, 2021, 148, 876-888.	2.9	9
58	Identification of ADGRE5 as discriminating MYC target between Burkitt lymphoma and diffuse large B-cell lymphoma. BMC Cancer, 2019, 19, 322.	2.6	8
59	Lactonization of the Oncometabolite D-2-Hydroxyglutarate Produces a Novel Endogenous Metabolite. Cancers, 2021, 13, 1756.	3.7	8
60	Cold Atmospheric Plasma Changes the Amino Acid Composition of Solutions and Influences the Anti-Tumor Effect on Melanoma Cells. International Journal of Molecular Sciences, 2021, 22, 7886.	4.1	8
61	Lower blood pH as a strong prognostic factor for fatal outcomes in critically ill COVID-19 patients at an intensive care unit: A multivariable analysis. PLoS ONE, 2021, 16, e0258018.	2.5	7
62	Synergy of interleukin 10 and toll‑like receptor 9 signalling in B cell proliferation: Implications for lymphoma pathogenesis. International Journal of Cancer, 2017, 140, 1147-1158.	5.1	5
63	Robust Metabolite Quantification from J-Compensated 2D 1H-13C-HSQC Experiments. Metabolites, 2020, 10, 449.	2.9	5
64	Validation Study for Non-Invasive Prediction of IDH Mutation Status in Patients with Glioma Using In Vivo 1H-Magnetic Resonance Spectroscopy and Machine Learning. Cancers, 2022, 14, 2762.	3.7	3
65	Overcoming the problems associated with poor spectra quality of the protein kinase Byr2 using residual dipolar couplings. Protein Science, 2001, 10, 1260-1263.	7.6	2
66	Protein-Protein Interaction Analysis by Docking. Algorithms, 2009, 2, 429-436.	2.1	2
67	Chemical shift optimization in multidimensional NMR spectra by AUREMOL-SHIFTOPT. Journal of Biomolecular NMR, 2009, 43, 197-210.	2.8	2
68	Evaluation of models for prognosing mortality in critical care patients with COVID-19: First- and second-wave data from a German university hospital. PLoS ONE, 2022, 17, e0268734.	2.5	1
69	Library Selection with a Randomized Repertoire of $(\beta\alpha)_8$-Barrel Enzymes Results in Unexpected Induction of Gene Expression. Biochemistry, 2019, 58, 4207-4217.	2.5	0
70	Assessment of Physiological Rat Kidney Ageing—Implications for the Evaluation of Allograft Quality Prior to Renal Transplantation. Metabolites, 2022, 12, 162.	2.9	0