

# Oliver Kohlbacher

## List of Publications by Year in descending order

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259  
papers

17,937  
citations

19608

61  
h-index

18606

119  
g-index

299  
all docs

299  
docs citations

299  
times ranked

28247  
citing authors

#	ARTICLE	IF	CITATIONS
1	Charting a dynamic DNA methylation landscape of the human genome. <i>Nature</i> , 2013, 500, 477-481.	13.7	1,168
2	Feature-based molecular networking in the GNPS analysis environment. <i>Nature Methods</i> , 2020, 17, 905-908.	9.0	650
3	Comprehensive Analysis of Alternative Splicing Across Tumors from 8,705 Patients. <i>Cancer Cell</i> , 2018, 34, 211-224.e6.	7.7	623
4	OptiType: precision HLA typing from next-generation sequencing data. <i>Bioinformatics</i> , 2014, 30, 3310-3316.	1.8	566
5	NRPSpredictor2—a web server for predicting NRPS adenylation domain specificity. <i>Nucleic Acids Research</i> , 2011, 39, W362-W367.	6.5	559
6	OpenMS — An open-source software framework for mass spectrometry. <i>BMC Bioinformatics</i> , 2008, 9, 163.	1.2	556
7	Visualization of omics data for systems biology. <i>Nature Methods</i> , 2010, 7, S56-S68.	9.0	548
8	OpenMS: a flexible open-source software platform for mass spectrometry data analysis. <i>Nature Methods</i> , 2016, 13, 741-748.	9.0	537
9	SARS-CoV-2-derived peptides define heterologous and COVID-19-induced T cell recognition. <i>Nature Immunology</i> , 2021, 22, 74-85.	7.0	490
10	Sequence co-evolution gives 3D contacts and structures of protein complexes. <i>ELife</i> , 2014, 3, .	2.8	452
11	Transcriptional and Epigenetic Dynamics during Specification of Human Embryonic Stem Cells. <i>Cell</i> , 2013, 153, 1149-1163.	13.5	419
12	Specificity prediction of adenylation domains in nonribosomal peptide synthetases (NRPS) using transductive support vector machines (TSVMs). <i>Nucleic Acids Research</i> , 2005, 33, 5799-5808.	6.5	388
13	MultiLoc: prediction of protein subcellular localization using N-terminal targeting sequences, sequence motifs and amino acid composition. <i>Bioinformatics</i> , 2006, 22, 1158-1165.	1.8	290
14	From hype to reality: data science enabling personalized medicine. <i>BMC Medicine</i> , 2018, 16, 150.	2.3	278
15	MultiLoc2: integrating phylogeny and Gene Ontology terms improves subcellular protein localization prediction. <i>BMC Bioinformatics</i> , 2009, 10, 274.	1.2	264
16	YLoc—an interpretable web server for predicting subcellular localization. <i>Nucleic Acids Research</i> , 2010, 38, W497-W502.	6.5	263
17	TOPP—the OpenMS proteomics pipeline. <i>Bioinformatics</i> , 2007, 23, e191-e197.	1.8	249
18	Photo-cross-linking and high-resolution mass spectrometry for assignment of RNA-binding sites in RNA-binding proteins. <i>Nature Methods</i> , 2014, 11, 1064-1070.	9.0	218

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19	Simultaneous alignment of short reads against multiple genomes. <i>Genome Biology</i> , 2009, 10, R98.	13.9	215
20	WIPI proteins: essential PtdIns3P effectors at the nascent autophagosome. <i>Journal of Cell Science</i> , 2015, 128, 207-17.	1.2	214
21	Tools for Label-free Peptide Quantification. <i>Molecular and Cellular Proteomics</i> , 2013, 12, 549-556.	2.5	198
22	Reentrant Condensation of Proteins in Solution Induced by Multivalent Counterions. <i>Physical Review Letters</i> , 2008, 101, 148101.	2.9	184
23	Immunoinformatics and epitope prediction in the age of genomic medicine. <i>Genome Medicine</i> , 2015, 7, 119.	3.6	178
24	The mzIdentML Data Standard for Mass Spectrometry-Based Proteomics Results. <i>Molecular and Cellular Proteomics</i> , 2012, 11, M111.014381-1-M111.014381-10.	2.5	175
25	Dissecting neural differentiation regulatory networks through epigenetic footprinting. <i>Nature</i> , 2015, 518, 355-359.	13.7	172
26	Elucidating the evolutionary conserved DNA-binding specificities of WRKY transcription factors by molecular dynamics and in vitro binding assays. <i>Nucleic Acids Research</i> , 2013, 41, 9764-9778.	6.5	161
27	The immunopeptidomic landscape of ovarian carcinomas. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E9942-E9951.	3.3	152
28	Recognizing millions of consistently unidentified spectra across hundreds of shotgun proteomics datasets. <i>Nature Methods</i> , 2016, 13, 651-656.	9.0	147
29	An Automated Pipeline for High-Throughput Label-Free Quantitative Proteomics. <i>Journal of Proteome Research</i> , 2013, 12, 1628-1644.	1.8	146
30	Going from where to why – interpretable prediction of protein subcellular localization. <i>Bioinformatics</i> , 2010, 26, 1232-1238.	1.8	133
31	The mzTab Data Exchange Format: Communicating Mass-spectrometry-based Proteomics and Metabolomics Experimental Results to a Wider Audience. <i>Molecular and Cellular Proteomics</i> , 2014, 13, 2765-2775.	2.5	130
32	HLA Ligand Atlas: a benign reference of HLA-presented peptides to improve T-cell-based cancer immunotherapy. , 2021, 9, e002071.		126
33	SherLoc2: A High-Accuracy Hybrid Method for Predicting Subcellular Localization of Proteins. <i>Journal of Proteome Research</i> , 2009, 8, 5363-5366.	1.8	122
34	SherLoc: high-accuracy prediction of protein subcellular localization by integrating text and protein sequence data. <i>Bioinformatics</i> , 2007, 23, 1410-1417.	1.8	113
35	Multi-omics discovery of exome-derived neoantigens in hepatocellular carcinoma. <i>Genome Medicine</i> , 2019, 11, 28.	3.6	107
36	Universality of protein reentrant condensation in solution induced by multivalent metal ions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 3450-3457.	1.5	106

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37	Genetic variation in human drug-related genes. <i>Genome Medicine</i> , 2017, 9, 117.	3.6	104
38	The antigenic landscape of multiple myeloma: mass spectrometry (re)defines targets for T-cell-based immunotherapy. <i>Blood</i> , 2015, 126, 1203-1213.	0.6	103
39	Interplay of pH and Binding of Multivalent Metal Ions: Charge Inversion and Reentrant Condensation in Protein Solutions. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5777-5787.	1.2	97
40	SANDPUMA: ensemble predictions of nonribosomal peptide chemistry reveal biosynthetic diversity across <i>Actinobacteria</i> . <i>Bioinformatics</i> , 2017, 33, 3202-3210.	1.8	89
41	Plants Release Precursors of Histone Deacetylase Inhibitors to Suppress Growth of Competitors. <i>Plant Cell</i> , 2015, 27, 3175-3189.	3.1	86
42	OpenMS – A platform for reproducible analysis of mass spectrometry data. <i>Journal of Biotechnology</i> , 2017, 261, 142-148.	1.9	85
43	Novel Formulation of Nonlocal Electrostatics. <i>Physical Review Letters</i> , 2004, 93, 108104.	2.9	83
44	Time-resolved characterization of cAMP/PKA-dependent signaling reveals that platelet inhibition is a concerted process involving multiple signaling pathways. <i>Blood</i> , 2014, 123, e1-e10.	0.6	80
45	Retention Time Prediction Improves Identification in Nontargeted Lipidomics Approaches. <i>Analytical Chemistry</i> , 2015, 87, 7698-7704.	3.2	80
46	SVMHC: a server for prediction of MHC-binding peptides. <i>Nucleic Acids Research</i> , 2006, 34, W194-W197.	6.5	79
47	POPISK: T-cell reactivity prediction using support vector machines and string kernels. <i>BMC Bioinformatics</i> , 2011, 12, 446.	1.2	79
48	Induction of neoantigen-reactive T cells from healthy donors. <i>Nature Protocols</i> , 2019, 14, 1926-1943.	5.5	78
49	Absolute Myoglobin Quantitation in Serum by Combining Two-Dimensional Liquid Chromatography- <sup>2</sup> Electrospray Ionization Mass Spectrometry and Novel Data Analysis Algorithms. <i>Journal of Proteome Research</i> , 2006, 5, 414-421.	1.8	77
50	Integrated modeling of the major events in the MHC class I antigen processing pathway. <i>Protein Science</i> , 2005, 14, 2132-2140.	3.1	76
51	Personalized peptide vaccine-induced immune response associated with long-term survival of a metastatic cholangiocarcinoma patient. <i>Journal of Hepatology</i> , 2016, 65, 849-855.	1.8	75
52	TOPPView: An Open-Source Viewer for Mass Spectrometry Data. <i>Journal of Proteome Research</i> , 2009, 8, 3760-3763.	1.8	74
53	Automated Label-free Quantification of Metabolites from Liquid Chromatography- <sup>2</sup> Mass Spectrometry Data. <i>Molecular and Cellular Proteomics</i> , 2014, 13, 348-359.	2.5	74
54	Prediction of dual protein targeting to plant organelles. <i>New Phytologist</i> , 2009, 183, 224-236.	3.5	73

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55	Data Integration for Future Medicine (DIFUTURE). <i>Methods of Information in Medicine</i> , 2018, 57, e57-e65.	0.7	73
56	Reduced Rate of Inpatient Hospital Admissions in 18 German University Hospitals During the COVID-19 Lockdown. <i>Frontiers in Public Health</i> , 2020, 8, 594117.	1.3	73
57	Statistical learning of peptide retention behavior in chromatographic separations: a new kernel-based approach for computational proteomics. <i>BMC Bioinformatics</i> , 2007, 8, 468.	1.2	70
58	GeneTrailExpress: a web-based pipeline for the statistical evaluation of microarray experiments. <i>BMC Bioinformatics</i> , 2008, 9, 552.	1.2	69
59	Activation of lymphoma-associated MyD88 mutations via allosterically-induced TIR-domain oligomerization. <i>Blood</i> , 2014, 124, 3896-3904.	0.6	69
60	PIA: An Intuitive Protein Inference Engine with a Web-Based User Interface. <i>Journal of Proteome Research</i> , 2015, 14, 2988-2997.	1.8	69
61	MetaRoute: fast search for relevant metabolic routes for interactive network navigation and visualization. <i>Bioinformatics</i> , 2008, 24, 2108-2109.	1.8	68
62	OpenMS and TOPP: Open Source Software for LC-MS Data Analysis. <i>Methods in Molecular Biology</i> , 2011, 696, 353-367.	0.4	68
63	Large-scale discovery of protein interactions at residue resolution using co-evolution calculated from genomic sequences. <i>Nature Communications</i> , 2021, 12, 1396.	5.8	68
64	The mzQuantML Data Standard for Mass Spectrometry-based Quantitative Studies in Proteomics. <i>Molecular and Cellular Proteomics</i> , 2013, 12, 2332-2340.	2.5	66
65	Structural and Functional Characterization of the Bacterial Type III Secretion Export Apparatus. <i>PLoS Pathogens</i> , 2016, 12, e1006071.	2.1	66
66	Copper oxide nanoparticle toxicity profiling using untargeted metabolomics. <i>Particle and Fibre Toxicology</i> , 2015, 13, 49.	2.8	65
67	MetaProSIP: Automated Inference of Stable Isotope Incorporation Rates in Proteins for Functional Metaproteomics. <i>Journal of Proteome Research</i> , 2015, 14, 619-627.	1.8	64
68	BALL - biochemical algorithms library 1.3. <i>BMC Bioinformatics</i> , 2010, 11, 531.	1.2	62
69	Distributed Analytics on Sensitive Medical Data: The Personal Health Train. <i>Data Intelligence</i> , 2020, 2, 96-107.	0.8	62
70	Food monitoring: Screening of the geographical origin of white asparagus using FT-NIR and machine learning. <i>Food Control</i> , 2019, 104, 318-325.	2.8	61
71	Modeling metabolic networks in <i>C. glutamicum</i> : a comparison of rate laws in combination with various parameter optimization strategies. <i>BMC Systems Biology</i> , 2009, 3, 5.	3.0	59
72	The MoSGrid Science Gateway - A Complete Solution for Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2232-2245.	2.3	58

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73	The HLA ligandome landscape of chronic myeloid leukemia delineates novel T-cell epitopes for immunotherapy. <i>Blood</i> , 2019, 133, 550-565.	0.6	57
74	In-depth analysis of protein inference algorithms using multiple search engines and well-defined metrics. <i>Journal of Proteomics</i> , 2017, 150, 170-182.	1.2	56
75	Mapping the HLA Ligandome of Colorectal Cancer Reveals an Imprint of Malignant Cell Transformation. <i>Cancer Research</i> , 2018, 78, 4627-4641.	0.4	56
76	The mzIdentML Data Standard Version 1.2, Supporting Advances in Proteome Informatics. <i>Molecular and Cellular Proteomics</i> , 2017, 16, 1275-1285.	2.5	55
77	A Combinatorial Approach to Protein Docking with Flexible Side Chains. <i>Journal of Computational Biology</i> , 2002, 9, 597-612.	0.8	54
78	A computational platform for high-throughput analysis of RNA sequences and modifications by mass spectrometry. <i>Nature Communications</i> , 2020, 11, 926.	5.8	54
79	BALLView: a tool for research and education in molecular modeling. <i>Bioinformatics</i> , 2006, 22, 365-366.	1.8	53
80	<i>De novo</i> peptide sequencing by tandem MS using complementary CID and electron transfer dissociation. <i>Electrophoresis</i> , 2009, 30, 3736-3747.	1.3	53
81	Machine learning competition in immunology – Prediction of HLA class I binding peptides. <i>Journal of Immunological Methods</i> , 2011, 374, 1-4.	0.6	53
82	BALLDock/SLICK: A New Method for Protein-Carbohydrate Docking. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1616-1625.	2.5	52
83	A novel algorithm for detecting differentially regulated paths based on gene set enrichment analysis. <i>Bioinformatics</i> , 2009, 25, 2787-2794.	1.8	51
84	TOPPAS: A Graphical Workflow Editor for the Analysis of High-Throughput Proteomics Data. <i>Journal of Proteome Research</i> , 2012, 11, 3914-3920.	1.8	50
85	Whither systems medicine?. <i>Experimental and Molecular Medicine</i> , 2018, 50, e453-e453.	3.2	49
86	Implications for selectivity of 3,4-diarylquinolinones as p38 $\beta$ -MAP kinase inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2008, 18, 1431-1435.	1.0	48
87	Learning from Heterogeneous Data Sources: An Application in Spatial Proteomics. <i>PLoS Computational Biology</i> , 2016, 12, e1004920.	1.5	47
88	A Fully Computational Model for Predicting Percutaneous Drug Absorption. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 424-429.	2.5	46
89	Automated scaffold selection for enzyme design. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 77, 74-83.	1.5	45
90	Probabilistic Consensus Scoring Improves Tandem Mass Spectrometry Peptide Identification. <i>Journal of Proteome Research</i> , 2011, 10, 3332-3343.	1.8	45

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91	A proteomics sample metadata representation for multiomics integration and big data analysis. <i>Nature Communications</i> , 2021, 12, 5854.	5.8	45
92	Computational modeling of the sugarâ€ˆlectin interaction. <i>Advanced Drug Delivery Reviews</i> , 2004, 56, 437-457.	6.6	43
93	LC-MSsim â€ˆ a simulation software for liquid chromatography mass spectrometry data. <i>BMC Bioinformatics</i> , 2008, 9, 423.	1.2	42
94	The role of phosphorylatable serine residues in the DNA-binding domain of Arabidopsis bZIP transcription factors. <i>European Journal of Cell Biology</i> , 2010, 89, 175-183.	1.6	42
95	qcML: An Exchange Format for Quality Control Metrics from Mass Spectrometry Experiments. <i>Molecular and Cellular Proteomics</i> , 2014, 13, 1905-1913.	2.5	42
96	HLA ligandome analysis of primary chronic lymphocytic leukemia (CLL) cells under lenalidomide treatment confirms the suitability of lenalidomide for combination with T-cell-based immunotherapy. <i>Oncolmmunology</i> , 2018, 7, e1316438.	2.1	42
97	Electrostatic potentials of proteins in water: a structured continuum approach. <i>Bioinformatics</i> , 2007, 23, e99-e103.	1.8	41
98	Using Atom Mapping Rules for an Improved Detection of Relevant Routes in Weighted Metabolic Networks. <i>Journal of Computational Biology</i> , 2008, 15, 565-576.	0.8	41
99	Designing string-of-beads vaccines with optimal spacers. <i>Genome Medicine</i> , 2016, 8, 9.	3.6	41
100	FLASHDeconv: Ultrafast, High-Quality Feature Deconvolution for Top-Down Proteomics. <i>Cell Systems</i> , 2020, 10, 213-218.e6.	2.9	41
101	BALLView: An object-oriented molecular visualization and modeling framework. <i>Journal of Computer-Aided Molecular Design</i> , 2005, 19, 791-800.	1.3	40
102	SLICK âˆ’ Scoring and Energy Functions for Proteinâˆ’Carbohydrate Interactions. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1635-1642.	2.5	40
103	Optimal de novo Design of MRM Experiments for Rapid Assay Development in Targeted Proteomics. <i>Journal of Proteome Research</i> , 2010, 9, 2696-2704.	1.8	40
104	Virtual screening and experimental validation reveal novel small-molecule inhibitors of 14-3-3 proteinâ€ˆprotein interactions. <i>Chemical Communications</i> , 2013, 49, 8468.	2.2	40
105	A Single Sign-On Infrastructure for Science Gateways on a Use Case for Structural Bioinformatics. <i>Journal of Grid Computing</i> , 2012, 10, 769-790.	2.5	39
106	Binding Pocket Optimization by Computational Protein Design. <i>PLoS ONE</i> , 2012, 7, e52505.	1.1	39
107	Comparative immunopeptidomics of humans and their pathogens. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 13268-13272.	3.3	38
108	Development of a fluorescence-based assay for screening of modulators of human Organic Anion Transporter 1B3 (OATP1B3). <i>European Journal of Pharmaceutics and Biopharmaceutics</i> , 2006, 62, 39-43.	2.0	38

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109	BNDDB – The Biochemical Network Database. BMC Bioinformatics, 2007, 8, 367.	1.2	36
110	Improving Peptide Identification in Proteome Analysis by a Two-Dimensional Retention Time Filtering Approach. Journal of Proteome Research, 2009, 8, 4109-4115.	1.8	36
111	Combining Structure and Sequence Information Allows Automated Prediction of Substrate Specificities within Enzyme Families. PLoS Computational Biology, 2010, 6, e1000636.	1.5	36
112	Universal peptide vaccines – Optimal peptide vaccine design based on viral sequence conservation. Vaccine, 2011, 29, 8745-8753.	1.7	35
113	Competing Salt Effects on Phase Behavior of Protein Solutions: Tailoring of Protein Interaction by the Binding of Multivalent Ions and Charge Screening. Journal of Physical Chemistry B, 2014, 118, 11365-11374.	1.2	35
114	MHCquant: Automated and Reproducible Data Analysis for Immunopeptidomics. Journal of Proteome Research, 2019, 18, 3876-3884.	1.8	35
115	Testing and Validation of Computational Methods for Mass Spectrometry. Journal of Proteome Research, 2016, 15, 809-814.	1.8	34
116	HIGH-ACCURACY PEAK PICKING OF PROTEOMICS DATA USING WAVELET TECHNIQUES. , 2005, , .		33
117	A Mathematical Framework for the Selection of an Optimal Set of Peptides for Epitope-Based Vaccines. PLoS Computational Biology, 2008, 4, e1000246.	1.5	32
118	OptiTope—a web server for the selection of an optimal set of peptides for epitope-based vaccines. Nucleic Acids Research, 2009, 37, W617-W622.	6.5	32
119	Workflows for automated downstream data analysis and visualization in large-scale computational mass spectrometry. Proteomics, 2015, 15, 1443-1447.	1.3	32
120	EpiToolKit—a web-based workbench for vaccine design. Bioinformatics, 2015, 31, 2211-2213.	1.8	32
121	FRED 2: an immunoinformatics framework for Python. Bioinformatics, 2016, 32, 2044-2046.	1.8	32
122	Identification of Ppar $\alpha$ -modulated miRNA hubs that target the fibrotic tumor microenvironment. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 454-463.	3.3	32
123	BiNA: A Visual Analytics Tool for Biological Network Data. PLoS ONE, 2014, 9, e87397.	1.1	31
124	Food Authentication: Small-Molecule Profiling as a Tool for the Geographic Discrimination of German White Asparagus. Journal of Agricultural and Food Chemistry, 2018, 66, 13328-13339.	2.4	31
125	Peak intensity prediction in MALDI-TOF mass spectrometry: A machine learning study to support quantitative proteomics. BMC Bioinformatics, 2008, 9, 443.	1.2	30
126	Novel Machine Learning Methods for MHC Class I Binding Prediction. Lecture Notes in Computer Science, 2010, , 98-109.	1.0	30



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127	Profile and Molecular Modeling of 3-(Indole-3-yl)-4-(3,4,5-trimethoxyphenyl)-1H-pyrrole-2,5-dione (1) as a Highly Selective VEGF-R2/3 Inhibitor. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 7549-7553.	2.9	29
128	LFQProfiler and RNPxl: Open-Source Tools for Label-Free Quantification and Protein-RNA Cross-Linking Integrated into Proteome Discoverer. <i>Journal of Proteome Research</i> , 2016, 15, 3441-3448.	1.8	29
129	Analysis of Genomic DNA from Medieval Plague Victims Suggests Long-Term Effect of <i>Yersinia pestis</i> on Human Immunity Genes. <i>Molecular Biology and Evolution</i> , 2021, 38, 4059-4076.	3.5	29
130	In melanoma, Hippo signaling is affected by copy number alterations and YAP1 overexpression impairs patient survival. <i>Pigment Cell and Melanoma Research</i> , 2014, 27, 671-673.	1.5	28
131	OpenMS and TOPP: Open Source Software for LC-MS Data Analysis. <i>Methods in Molecular Biology</i> , 2010, 604, 201-211.	0.4	27
132	Lectin-sugar interaction. <i>FEBS Journal</i> , 2002, 269, 1518-1524.	0.2	26
133	SNEP: SNP-derived Epitope Prediction program for minor H antigens. <i>Immunogenetics</i> , 2005, 57, 816-820.	1.2	26
134	Comparison of different sample preparation techniques for NIR screening and their influence on the geographical origin determination of almonds ( <i>Prunus dulcis</i> MILL.). <i>Food Control</i> , 2020, 115, 107302.	2.8	26
135	Analysis of protein-RNA interactions in CRISPR proteins and effector complexes by UV-induced cross-linking and mass spectrometry. <i>Methods</i> , 2015, 89, 138-148.	1.9	25
136	Data Management of Sensitive Human Proteomics Data: Current Practices, Recommendations, and Perspectives for the Future. <i>Molecular and Cellular Proteomics</i> , 2021, 20, 100071.	2.5	25
137	A statistical learning approach to the modeling of chromatographic retention of oligonucleotides incorporating sequence and secondary structure data. <i>Nucleic Acids Research</i> , 2007, 35, 4195-4202.	6.5	23
138	DNA-binding proteins from marine bacteria expand the known sequence diversity of TALE-like repeats. <i>Nucleic Acids Research</i> , 2015, 43, gkv1053.	6.5	23
139	Scaling home automation to public buildings: A distributed multiuser setup for OpenHAB 2., 2017, .		23
140	SmartPeak Automates Targeted and Quantitative Metabolomics Data Processing. <i>Analytical Chemistry</i> , 2020, 92, 15968-15974.	3.2	23
141	Application of displacement chromatography for the proteome analysis of a human plasma protein fraction. <i>Journal of Chromatography A</i> , 2010, 1217, 3321-3329.	1.8	22
142	An unusually high substitution rate in transplant-associated BK polyomavirus in vivo is further concentrated in HLA-C-bound viral peptides. <i>PLoS Pathogens</i> , 2018, 14, e1007368.	2.1	22
143	Challenges of big data integration in the life sciences. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 6791-6800.	1.9	22
144	Multiple Layers of Phospho-Regulation Coordinate Metabolism and the Cell Cycle in Budding Yeast. <i>Frontiers in Cell and Developmental Biology</i> , 2019, 7, 338.	1.8	22

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145	Analysis of protein-DNA interactions in chromatin by UV induced cross-linking and mass spectrometry. <i>Nature Communications</i> , 2020, 11, 5250.	5.8	22
146	High-accuracy peak picking of proteomics data using wavelet techniques. <i>Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing</i> , 2006, , 243-54.	0.7	22
147	From sequence to structure and back again: approaches for predicting protein-DNA binding. <i>Proteome Science</i> , 2004, 2, 3.	0.7	21
148	Structure-Activity Relationships in Chromatography: Retention Prediction of Oligonucleotides with Support Vector Regression. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 7009-7012.	7.2	21
149	EpiToolKit—a web server for computational immunomics. <i>Nucleic Acids Research</i> , 2008, 36, W519-W522.	6.5	21
150	KIRMES: kernel-based identification of regulatory modules in euchromatic sequences. <i>Bioinformatics</i> , 2009, 25, 2126-2133.	1.8	21
151	Protein (multi-)location prediction: utilizing interdependencies via a generative model. <i>Bioinformatics</i> , 2015, 31, i365-i374.	1.8	21
152	Food authentication: Determination of the geographical origin of almonds ( <i>Prunus dulcis</i> Mill.) via near-infrared spectroscopy. <i>Microchemical Journal</i> , 2021, 160, 105702.	2.3	21
153	FRED—a framework for T-cell epitope detection. <i>Bioinformatics</i> , 2009, 25, 2758-2759.	1.8	20
154	Carfilzomib alters the HLA-presented peptidome of myeloma cells and impairs presentation of peptides with aromatic C-termini. <i>Blood Cancer Journal</i> , 2016, 6, e411-e411.	2.8	20
155	Untargeted Metabolomics Reveals Molecular Effects of Ketogenic Diet on Healthy and Tumor Xenograft Mouse Models. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3873.	1.8	20
156	EPIFANY: A Method for Efficient High-Confidence Protein Inference. <i>Journal of Proteome Research</i> , 2020, 19, 1060-1072.	1.8	20
157	Genome-wide study of a Neolithic Wartberg grave community reveals distinct HLA variation and hunter-gatherer ancestry. <i>Communications Biology</i> , 2021, 4, 113.	2.0	20
158	Computational proteomics pitfalls and challenges: HavanaBioinfo 2012 Workshop report. <i>Journal of Proteomics</i> , 2013, 87, 134-138.	1.2	19
159	Mass-Spectrometry-Based Proteomics Reveals Organ-Specific Expression Patterns To Be Used as Forensic Evidence. <i>Journal of Proteome Research</i> , 2016, 15, 182-192.	1.8	19
160	Determination of the Geographical Origin of <i>Asparagus officinalis</i> L. by <sup>1</sup> H NMR Spectroscopy. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 14353-14363.	2.4	19
161	Multiple Instance Learning Allows MHC Class II Epitope Predictions Across Alleles. <i>Lecture Notes in Computer Science</i> , 2008, , 210-221.	1.0	19
162	The future of metabolomics in ELIXIR. <i>F1000Research</i> , 2017, 6, 1649.	0.8	19

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163	Towards <i>in silico</i> design of epitope-based vaccines. <i>Expert Opinion on Drug Discovery</i> , 2009, 4, 1047-1060.	2.5	18
164	Covalent attachment of pyridoxal-phosphate derivatives to 14-3-3 proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, E1051-3; author reply E1054.	3.3	18
165	Distinct transcriptional changes in non-small cell lung cancer patients associated with multi-antigenic RNAActive® CV9201 immunotherapy. <i>Oncolmunology</i> , 2016, 5, e1249560.	2.1	18
166	Improving global feature detectabilities through scan range splitting for untargeted metabolomics by high-performance liquid chromatography-Orbitrap mass spectrometry. <i>Analytica Chimica Acta</i> , 2016, 930, 13-22.	2.6	18
167	qPortal: A platform for data-driven biomedical research. <i>PLoS ONE</i> , 2018, 13, e0191603.	1.1	18
168	BN++ – A Biological Information System. <i>Journal of Integrative Bioinformatics</i> , 2006, 3, 148-161.	1.0	17
169	Exploiting physico-chemical properties in string kernels. <i>BMC Bioinformatics</i> , 2010, 11, S7.	1.2	17
170	Fluorescence-based imaging of autophagy progression by human WIPI protein detection. <i>Methods</i> , 2015, 75, 69-78.	1.9	17
171	Clinical and non-targeted metabolomic profiling of homozygous carriers of Transcription Factor 7-like 2 variant rs7903146. <i>Scientific Reports</i> , 2014, 4, 5296.	1.6	17
172	The Endometrial Transcription Landscape of MRKH Syndrome. <i>Frontiers in Cell and Developmental Biology</i> , 2020, 8, 572281.	1.8	17
173	DIAproteomics: A Multifunctional Data Analysis Pipeline for Data-Independent Acquisition Proteomics and Peptidomics. <i>Journal of Proteome Research</i> , 2021, 20, 3758-3766.	1.8	17
174	Structure prediction of protein complexes by an NMR-based protein docking algorithm. <i>Journal of Biomolecular NMR</i> , 2001, 20, 15-21.	1.6	16
175	No Longer Confidential: Estimating the Confidence of Individual Regression Predictions. <i>PLoS ONE</i> , 2012, 7, e48723.	1.1	16
176	Displacement chromatography as first separating step in online two-dimensional liquid chromatography coupled to mass spectrometry analysis of a complex protein sample – The proteome of neutrophils. <i>Journal of Chromatography A</i> , 2012, 1232, 288-294.	1.8	16
177	Population-specific design of de-immunized protein biotherapeutics. <i>PLoS Computational Biology</i> , 2018, 14, e1005983.	1.5	16
178	Understanding the constitutive presentation of MHC class I immunopeptidomes in primary tissues. <i>IScience</i> , 2022, 25, 103768.	1.9	16
179	Epitope prediction algorithms for peptide-based vaccine design. <i>Proceedings</i> , 2003, 2, 17-26.	0.1	16
180	Population Genetics and Signatures of Selection in Early Neolithic European Farmers. <i>Molecular Biology and Evolution</i> , 2022, 39, .	3.5	16

#	ARTICLE	IF	CITATIONS
181	Food fingerprinting: Mass spectrometric determination of the cocoa shell content ( <i>Theobroma cacao</i> ) Tj ETQq1 1 0,784314 rgBT /Overl	4.2	14
182	Annotation and initial evaluation of a large annotated German oncological corpus. <i>JAMIA Open</i> , 2021, 4, ooab025.	1.0	14
183	The bifunctional role of aconitase in <i>S</i> treptomyces viridochromogenes. <i>Environmental Microbiology</i> , 2012, 14, 3203-3219.	1.8	13
184	Identification of HCMV-derived T cell epitopes in seropositive individuals through viral deletion models. <i>Journal of Experimental Medicine</i> , 2020, 217, .	4.2	13
185	A community proposal to integrate proteomics activities in ELIXIR. <i>F1000Research</i> , 2017, 6, 875.	0.8	13
186	Exploring protein-protein interactions at the proteome level. <i>Structure</i> , 2022, 30, 462-475.	1.6	13
187	From the desktop to the grid: scalable bioinformatics via workflow conversion. <i>BMC Bioinformatics</i> , 2016, 17, 127.	1.2	12
188	A meta-analysis of HLA peptidome composition in different hematological entities: entity-specific dividing lines and <i>pan-leukemia</i> antigens. <i>Oncotarget</i> , 2017, 8, 43915-43924.	0.8	12
189	The COVID-19 Data Exchange Platform of the German University Medicine. <i>Studies in Health Technology and Informatics</i> , 2022, , .	0.2	12
190	SIGNIFICANTLY IMPROVED PREDICTION OF SUBCELLULAR LOCALIZATION BY INTEGRATING TEXT AND PROTEIN SEQUENCE DATA. , 2005, , .		11
191	ClinOmicsTrailbc: a visual analytics tool for breast cancer treatment stratification. <i>Bioinformatics</i> , 2019, 35, 5171-5181.	1.8	11
192	The future of metabolomics in ELIXIR. <i>F1000Research</i> , 2017, 6, 1649.	0.8	11
193	DIAMetAlyzer allows automated false-discovery rate-controlled analysis for data-independent acquisition in metabolomics. <i>Nature Communications</i> , 2022, 13, 1347.	5.8	11
194	Dithiothreitol (DTT) Acts as a Specific, UV-inducible Cross-linker in Elucidation of Proteinâ€“RNA Interactions*. <i>Molecular and Cellular Proteomics</i> , 2015, 14, 3196-3210.	2.5	10
195	Nephron Toxicity Profiling via Untargeted Metabolome Analysis Employing a High Performance Liquid Chromatography-Mass Spectrometry-based Experimental and Computational Pipeline. <i>Journal of Biological Chemistry</i> , 2015, 290, 19121-19132.	1.6	10
196	ballaxy: web services for structural bioinformatics. <i>Bioinformatics</i> , 2015, 31, 121-122.	1.8	10
197	OpenPepXL: An Open-Source Tool for Sensitive Identification of Cross-Linked Peptides in XL-MS. <i>Molecular and Cellular Proteomics</i> , 2020, 19, 2157-2168.	2.5	10
198	Integrative analysis of cancerâ€“related data using CAP. <i>FASEB Journal</i> , 2004, 18, 1465-1467.	0.2	9

#	ARTICLE	IF	CITATIONS
199	In silico design of targeted SRM-based experiments. BMC Bioinformatics, 2012, 13, S8.	1.2	9
200	Blocked Inverted Indices for Exact Clustering of Large Chemical Spaces. Journal of Chemical Information and Modeling, 2014, 54, 2395-2401.	2.5	9
201	CADDSuite – a workflow-enabled suite of open-source tools for drug discovery. Journal of Cheminformatics, 2012, 4, .	2.8	8
202	Performance Studies on Distributed Virtual Screening. BioMed Research International, 2014, 2014, 1-7.	0.9	8
203	DrugTargetInspector: An assistance tool for patient treatment stratification. International Journal of Cancer, 2016, 138, 1765-1776.	2.3	8
204	Proteins and Molecular Pathways Relevant for the Malignant Properties of Tumor-Initiating Pancreatic Cancer Cells. Cells, 2020, 9, 1397.	1.8	8
205	Application of displacement chromatography for the analysis of a lipid raft proteome. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2010, 878, 309-314.	1.2	7
206	Improved particle-packed HPLC/MS microchips for proteomic analysis. Journal of Separation Science, 2010, 33, 3283-3291.	1.3	7
207	miHA-Match: Computational detection of tissue-specific minor histocompatibility antigens. Journal of Immunological Methods, 2012, 386, 94-100.	0.6	7
208	Phosphoproteomics of short-term hedgehog signaling in human medulloblastoma cells. Cell Communication and Signaling, 2020, 18, 99.	2.7	7
209	Tracing incorporation of heavy water into proteins for species-specific metabolic activity in complex communities. Journal of Proteomics, 2020, 222, 103791.	1.2	7
210	Genetic authentication: Differentiation of hazelnut cultivars using polymorphic sites of the chloroplast genome. Food Control, 2021, 130, 108344.	2.8	7
211	Interpretation of the DOME Recommendations for Machine Learning in Proteomics and Metabolomics. Journal of Proteome Research, 2022, 21, 1204-1207.	1.8	7
212	ImmunoNodes – graphical development of complex immunoinformatics workflows. BMC Bioinformatics, 2017, 18, 242.	1.2	6
213	Patient Empowerment During the COVID-19 Pandemic by Ensuring Safe and Fast Communication of Test Results: Implementation and Performance of a Tracking System. Journal of Medical Internet Research, 2021, 23, e27348.	2.1	6
214	Metabolomics Data Processing Using OpenMS. Methods in Molecular Biology, 2020, 2104, 49-60.	0.4	6
215	T-cell epitope prediction based on self-tolerance. , 2011, , .		5
216	PTMeta: Increasing identification rates of modified peptides using modification prescanning and meta-analysis. Proteomics, 2013, 13, 1042-1051.	1.3	5

#	ARTICLE	IF	CITATIONS
217	Managing Expectations When Publishing Tools and Methods for Computational Proteomics. Journal of Proteome Research, 2015, 14, 2002-2004.	1.8	5
218	Reproducible Scientific Workflows for High Performance and Cloud Computing. , 2019, , .		5
219	BALL: Biochemical Algorithms Library. Lecture Notes in Computer Science, 1999, , 330-344.	1.0	5
220	Integer Linear Programming in Computational Biology. Lecture Notes in Computer Science, 2009, , 199-218.	1.0	5
221	Efficient privacy-preserving whole-genome variant queries. Bioinformatics, 2022, 38, 2202-2210.	1.8	5
222	Bioinformatics for Qualitative and Quantitative Proteomics. Methods in Molecular Biology, 2011, 719, 331-349.	0.4	4
223	No evidence of viral genomes in whole-€transcriptome sequencing of three melanoma metastases. Experimental Dermatology, 2011, 20, 766-768.	1.4	4
224	On Comparison of SimTandem with State-of-the-Art Peptide Identification Tools, Efficiency of Precursor Mass Filter and Dealing with Variable Modifications. Journal of Integrative Bioinformatics, 2013, 10, 1-15.	1.0	4
225	Favorable immune signature in CLL patients, defined by antigen-specific T-cell responses, might prevent second skin cancers. Leukemia and Lymphoma, 2018, 59, 1949-1958.	0.6	4
226	ClinVAP: a reporting strategy from variants to therapeutic options. Bioinformatics, 2020, 36, 2316-2317.	1.8	4
227	Algorithms for the Automated Absolute Quantification of Diagnostic Markers in Complex Proteomics Samples. Lecture Notes in Computer Science, 2005, , 151-162.	1.0	4
228	Comparison of displacement versus gradient mode for separation of a complex protein mixture by anion-exchange chromatography. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2012, 901, 34-40.	1.2	3
229	Intuitive Web-Based Experimental Design for High-Throughput Biomedical Data. BioMed Research International, 2015, 2015, 1-8.	0.9	3
230	Novel Visual Metaphors for Multivariate Networks. Lecture Notes in Computer Science, 2014, , 127-150.	1.0	3
231	The de.NBI / ELIXIR-DE training platform - Bioinformatics training in Germany and across Europe within ELIXIR. F1000Research, 2019, 8, 1877.	0.8	3
232	Modeling Protein-Protein and Protein-DNA Docking. , 0, , 601-650.		2
233	Analysis of MHC-Peptide Binding Using Amino Acid Property-Based Decision Rules. Lecture Notes in Computer Science, 2005, , 446-453.	1.0	2
234	Workflow-enhanced conformational analysis of guanidine zinc complexes via a science gateway. Studies in Health Technology and Informatics, 2012, 175, 142-51.	0.2	2

#	ARTICLE	IF	CITATIONS
235	Visualising Metabolic Pathways and Networks: Past, Present, Future. , 2022, , 237-267.		2
236	MoSGrid â€“ a molecular simulation grid as a new tool in computational chemistry, biology and material science. Journal of Cheminformatics, 2011, 3, .	2.8	1
237	Rebuilding KEGG Maps: Algorithms and Benefits. , 2014, , .		1
238	Differential Enzymatic <sup>16</sup> O/ <sup>18</sup> O Labeling for the Detection of Cross-Linked Nucleic Acidâ€™Protein Heteroconjugates. Analytical Chemistry, 2017, 89, 11208-11213.	3.2	1
239	Enabling ad-hoc reuse of private data repositories through schema extraction. Journal of Biomedical Semantics, 2020, 11, 6.	0.9	1
240	Abstract B124: Personalized peptide vaccination based on patient-individual tumor-specific variants induces T-cell responses in pediatric patients. Cancer Immunology Research, 2019, 7, B124-B124.	1.6	1
241	The de.NBI / ELIXIR-DE training platform - Bioinformatics training in Germany and across Europe within ELIXIR. F1000Research, 2019, 8, 1877.	0.8	1
242	A Statistical Comparison of SimTandem with State-of-the-Art Peptide Identification Tools. Advances in Intelligent Systems and Computing, 2013, , 101-109.	0.5	1
243	Abstract CT057: Phase I trial to evaluate the feasibility and safety of an individualized peptide vaccine of unmodified cancer antigens: PepIVAC-01. , 2018, , .		1
244	Interactive Visualization for Large-Scale Multi-factorial Research Designs. Lecture Notes in Computer Science, 2019, , 75-84.	1.0	1
245	De novo identification of maximally deregulated subnetworks based on multi-omics data with DeRegNet. BMC Bioinformatics, 2022, 23, 139.	1.2	1
246	On comparison of SimTandem with state-of-the-art peptide identification tools, efficiency of precursor mass filter and dealing with variable modifications. Journal of Integrative Bioinformatics, 2013, 10, 228.	1.0	1
247	TOPP goes Rapid The OpenMS Proteomics Pipeline in a Grid-Enabled Web Portal. , 2010, , .		0
248	Molecular simulation grid. Journal of Cheminformatics, 2011, 3, .	2.8	0
249	A framework and workflow system for virtual screening and molecular docking. Journal of Cheminformatics, 2011, 3, .	2.8	0
250	miHA-match. , 2012, , .		0
251	Network-based interactive navigation and analysis of large biological datasets. IT - Information Technology, 2015, 57, 37-48.	0.6	0
252	BALL-SNPgâ€™from genetic variants toward computational diagnostics. Bioinformatics, 2016, 32, 1888-1890.	1.8	0

#	ARTICLE	IF	CITATIONS
253	Challenges in Large-Scale Computational Mass Spectrometry and Multiomics. Journal of Proteome Research, 2016, 15, 681-682.	1.8	0
254	BOOTABLE: Bioinformatics Benchmark Tool Suite. , 2019, , .		0
255	Interplay Between the Immune System and Colorectal Carcinoma - Towards Tumor-Specific Peptide-Based Vaccination for Any HLA-Type. Blood, 2015, 126, 1027-1027.	0.6	0
256	Abstract A113: iVacALL: A personalized peptide-vaccination design platform for pediatric acute lymphoblastic leukemia patients based on patient-individual tumor-specific variants. , 2016, , .		0
257	Abstract A112: Mapping the impact of proteasome inhibitor therapy on the antigenic landscape of multiple myeloma: Identifying robust targets for T cell immunotherapy. , 2016, , .		0
258	Unique Alterations in the Immunopeptidome of Colorectal Cancer Reflect Specific Transformations in Cancer-Associated Signaling Pathways and Reveal Tumor-Specific HLA-Ligand Modulations. Blood, 2016, 128, 862-862.	0.6	0
259	The HLA Ligandome Landscape of Chronic Myeloid Leukemia Delineates Novel T-Cell Epitopes for Immunotherapy. Blood, 2018, 132, 4243-4243.	0.6	0