Oliver Kohlbacher

List of Publications by Year
in descending order

259 papers	17,937 citations	19657 61 h-index	18647 119 g-index
299 all docs	299 docs citations	299 times ranked	28247 citing authors

#	Article	IF	Citations
1	Understanding the constitutive presentation of MHC class I immunopeptidomes in primary tissues. IScience, 2022, 25, 103768.	4.1	16
2	Efficient privacy-preserving whole-genome variant queries. Bioinformatics, 2022, 38, 2202-2210.	4.1	5
3	Interpretation of the DOME Recommendations for Machine Learning in Proteomics and Metabolomics. Journal of Proteome Research, 2022, 21, 1204-1207.	3.7	7
4	DIAMetAlyzer allows automated false-discovery rate-controlled analysis for data-independent acquisition in metabolomics. Nature Communications, 2022, 13, 1347.	12.8	11
5	Exploring protein-protein interactions at the proteome level. Structure, 2022, 30, 462-475.	3.3	13
6	Visualising Metabolic Pathways and Networks: Past, Present, Future. , 2022, , 237-267.		2
7	De novo identification of maximally deregulated subnetworks based on multi-omics data with DeRegNet. BMC Bioinformatics, 2022, 23, 139.	2.6	1
8	Population Genetics and Signatures of Selection in Early Neolithic European Farmers. Molecular Biology and Evolution, 2022, 39, .	8.9	16
9	The COVID-19 Data Exchange Platform of the German University Medicine. Studies in Health Technology and Informatics, 2022, , .	0.3	12
10	SARS-CoV-2-derived peptides define heterologous and COVID-19-induced T cell recognition. Nature Immunology, 2021, 22, 74-85.	14.5	490
11	Food authentication: Determination of the geographical origin of almonds (Prunus dulcis Mill.) via near-infrared spectroscopy. Microchemical Journal, 2021, 160, 105702.	4.5	21
12	Genome-wide study of a Neolithic Wartberg grave community reveals distinct HLA variation and hunter-gatherer ancestry. Communications Biology, 2021, 4, 113.	4.4	20
13	Data Management of Sensitive Human Proteomics Data: Current Practices, Recommendations, and Perspectives for the Future. Molecular and Cellular Proteomics, 2021, 20, 100071.	3.8	25
14	Large-scale discovery of protein interactions at residue resolution using co-evolution calculated from genomic sequences. Nature Communications, 2021, 12, 1396.	12.8	68
15	HLA Ligand Atlas: a benign reference of HLA-presented peptides to improve T-cell-based cancer immunotherapy. , 2021, 9, e002071.		126
16	Annotation and initial evaluation of a large annotated German oncological corpus. JAMIA Open, 2021, 4, ooab025.	2.0	14
17	Analysis of Genomic DNA from Medieval Plague Victims Suggests Long-Term Effect of <i>Yersinia pestis</i> on Human Immunity Genes. Molecular Biology and Evolution, 2021, 38, 4059-4076.	8.9	29
18	DIAproteomics: A Multifunctional Data Analysis Pipeline for Data-Independent Acquisition Proteomics and Peptidomics. Journal of Proteome Research, 2021, 20, 3758-3766.	3.7	17

#	Article	IF	Citations
19	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.	4.3	6
20	Genetic authentication: Differentiation of hazelnut cultivars using polymorphic sites of the chloroplast genome. Food Control, 2021, 130, 108344.	5.5	7
21	A proteomics sample metadata representation for multiomics integration and big data analysis. Nature Communications, 2021, 12, 5854.	12.8	45
22	ClinVAP: a reporting strategy from variants to therapeutic options. Bioinformatics, 2020, 36, 2316-2317.	4.1	4
23	Distributed Analytics on Sensitive Medical Data: The Personal Health Train. Data Intelligence, 2020, 2, 96-107.	1.5	62
24	Analysis of protein-DNA interactions in chromatin by UV induced cross-linking and mass spectrometry. Nature Communications, 2020, 11, 5250.	12.8	22
25	The Endometrial Transcription Landscape of MRKH Syndrome. Frontiers in Cell and Developmental Biology, 2020, 8, 572281.	3.7	17
26	SmartPeak Automates Targeted and Quantitative Metabolomics Data Processing. Analytical Chemistry, 2020, 92, 15968-15974.	6.5	23
27	Identification of HCMV-derived T cell epitopes in seropositive individuals through viral deletion models. Journal of Experimental Medicine, 2020, 217, .	8.5	13
28	Determination of the Geographical Origin of *Asparagus officinalis* L. by ^{1}H NMR Spectroscopy. Journal of Agricultural and Food Chemistry, 2020, 68, 14353-14363.	5.2	19
29	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	19.0	650
30	Proteins and Molecular Pathways Relevant for the Malignant Properties of Tumor-Initiating Pancreatic Cancer Cells. Cells, 2020, 9, 1397.	4.1	8
31	Phosphoproteomics of short-term hedgehog signaling in human medulloblastoma cells. Cell Communication and Signaling, 2020, 18, 99.	6.5	7
32	Enabling ad-hoc reuse of private data repositories through schema extraction. Journal of Biomedical Semantics, 2020, 11, 6.	1.6	1
33	Identification of Ppar *γ* -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.	7.1	32
34	FLASHDeconv: Ultrafast, High-Quality Feature Deconvolution for Top-Down Proteomics. Cell Systems, 2020, 10, 213-218.e6.	6.2	41
35	EPIFANY: A Method for Efficient High-Confidence Protein Inference. Journal of Proteome Research, 2020, 19, 1060-1072.	3.7	20
36	Tracing incorporation of heavy water into proteins for species-specific metabolic activity in complex communities. Journal of Proteomics, 2020, 222, 103791.	2.4	7

#	Article	IF	Citations
37	Comparison of different sample preparation techniques for NIR screening and their influence on the geographical origin determination of almonds (Prunus dulcis MILL.). Food Control, 2020, 115, 107302.	5.5	26
38	Reduced Rate of Inpatient Hospital Admissions in 18 German University Hospitals During the COVID-19 Lockdown. Frontiers in Public Health, 2020, 8, 594117.	2.7	73
39	Metabolomics Data Processing Using OpenMS. Methods in Molecular Biology, 2020, 2104, 49-60.	0.9	6
40	A computational platform for high-throughput analysis of RNA sequences and modifications by mass spectrometry. Nature Communications, 2020, 11, 926.	12.8	54
41	OpenPepXL: An Open-Source Tool for Sensitive Identification of Cross-Linked Peptides in XL-MS. Molecular and Cellular Proteomics, 2020, 19, 2157-2168.	3.8	10
42	Untargeted Metabolomics Reveals Molecular Effects of Ketogenic Diet on Healthy and Tumor Xenograft Mouse Models. International Journal of Molecular Sciences, 2019, 20, 3873.	4.1	20
43	Reproducible Scientific Workflows for High Performance and Cloud Computing. , 2019, , .		5
44	BOOTABLE: Bioinformatics Benchmark Tool Suite. , 2019, , .		0
45	MHCquant: Automated and Reproducible Data Analysis for Immunopeptidomics. Journal of Proteome Research, 2019, 18, 3876-3884.	3.7	35
46	Challenges of big data integration in the life sciences. Analytical and Bioanalytical Chemistry, 2019, 411, 6791-6800.	3.7	22
47	Food fingerprinting: Mass spectrometric determination of the cocoa shell content (Theobroma cacao) Tj ETQq1 1 0.784314 rgBT /Ove	8.2	14
48	Induction of neoantigen-reactive T cells from healthy donors. Nature Protocols, 2019, 14, 1926-1943.	12.0	78
49	Multi-omics discovery of exome-derived neoantigens in hepatocellular carcinoma. Genome Medicine, 2019, 11, 28.	8.2	107
50	Food monitoring: Screening of the geographical origin of white asparagus using FT-NIR and machine learning. Food Control, 2019, 104, 318-325.	5.5	61
51	ClinOmicsTrailbc: a visual analytics tool for breast cancer treatment stratification. Bioinformatics, 2019, 35, 5171-5181.	4.1	11
52	Multiple Layers of Phospho-Regulation Coordinate Metabolism and the Cell Cycle in Budding Yeast. Frontiers in Cell and Developmental Biology, 2019, 7, 338.	3.7	22
53	The HLA ligandome landscape of chronic myeloid leukemia delineates novel T-cell epitopes for immunotherapy. Blood, 2019, 133, 550-565.	1.4	57
54	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.	3.4	1

#	Article	IF	Citations
55	The de.NBI / ELIXIR-DE training platform - Bioinformatics training in Germany and across Europe within ELIXIR. F1000Research, 2019, 8, 1877.	1.6	1
56	Interactive Visualization for Large-Scale Multi-factorial Research Designs. Lecture Notes in Computer Science, 2019, , 75-84.	1.3	1
57	The de.NBI / ELIXIR-DE training platform - Bioinformatics training in Germany and across Europe within ELIXIR. F1000Research, 2019, 8, 1877.	1.6	3
58	Whither systems medicine?. Experimental and Molecular Medicine, 2018, 50, e453-e453.	7.7	49
59	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.	1.3	4
60	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. OncoImmunology, 2018, 7, e1316438.	4.6	42
61	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.	5.2	31
62	An unusually high substitution rate in transplant-associated BK polyomavirus in vivo is further concentrated in HLA-C-bound viral peptides. PLoS Pathogens, 2018, 14, e1007368.	4.7	22
63	Mapping the HLA Ligandome of Colorectal Cancer Reveals an Imprint of Malignant Cell Transformation. Cancer Research, 2018, 78, 4627-4641.	0.9	56
64	Comprehensive Analysis of Alternative Splicing Across Tumors from 8,705 Patients. Cancer Cell, 2018, 34, 211-224.e6.	16.8	623
65	Data Integration for Future Medicine (DIFUTURE). Methods of Information in Medicine, 2018, 57, e57-e65.	1.2	73
66	From hype to reality: data science enabling personalized medicine. BMC Medicine, 2018, 16, 150.	5.5	278
67	Population-specific design of de-immunized protein biotherapeutics. PLoS Computational Biology, 2018, 14, e1005983.	3.2	16
68	qPortal: A platform for data-driven biomedical research. PLoS ONE, 2018, 13, e0191603.	2.5	18
69	Abstract CT057: Phase I trial to evaluate the feasibility and safety of an individualized peptide vaccine of unmodified cancer antigens: PepIVAC-01. , 2018, , .		1
70	The HLA Ligandome Landscape of Chronic Myeloid Leukemia Delineates Novel T-Cell Epitopes for Immunotherapy. Blood, 2018, 132, 4243-4243.	1.4	0
71	SANDPUMA: ensemble predictions of nonribosomal peptide chemistry reveal biosynthetic diversity across <i>Actinobacteria</i>. Bioinformatics, 2017, 33, 3202-3210.	4.1	89
72	OpenMS â€" A platform for reproducible analysis of mass spectrometry data. Journal of Biotechnology, 2017, 261, 142-148.	3.8	85

#	Article	IF	Citations
73	Scaling home automation to public buildings: A distributed multiuser setup for OpenHAB 2. , 2017, , .		23
74	Differential Enzymatic ^{16}O/^{18}O Labeling for the Detection of Cross-Linked Nucleic Acid–Protein Heteroconjugates. Analytical Chemistry, 2017, 89, 11208-11213.	6.5	1
75	The immunopeptidomic landscape of ovarian carcinomas. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E9942-E9951.	7.1	152
76	ImmunoNodes – graphical development of complex immunoinformatics workflows. BMC Bioinformatics, 2017, 18, 242.	2.6	6
77	The mzIdentML Data Standard Version 1.2, Supporting Advances in Proteome Informatics. Molecular and Cellular Proteomics, 2017, 16, 1275-1285.	3.8	55
78	In-depth analysis of protein inference algorithms using multiple search engines and well-defined metrics. Journal of Proteomics, 2017, 150, 170-182.	2.4	56
79	Genetic variation in human drug-related genes. Genome Medicine, 2017, 9, 117.	8.2	104
80	A community proposal to integrate proteomics activities in ELIXIR. F1000Research, 2017, 6, 875.	1.6	13
81	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	1.6	19
82	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	1.6	11
83	A meta-analysis of HLA peptidome composition in different hematological entities: entity-specific dividing lines and "pan-leukemia" antigens. Oncotarget, 2017, 8, 43915-43924.	1.8	12
84	DrugTargetInspector: An assistance tool for patient treatment stratification. International Journal of Cancer, 2016, 138, 1765-1776.	5.1	8
85	Personalized peptide vaccine-induced immune response associated with long-term survival of a metastatic cholangiocarcinoma patient. Journal of Hepatology, 2016, 65, 849-855.	3.7	75
86	Carfilzomib alters the HLA-presented peptidome of myeloma cells and impairs presentation of peptides with aromatic C-termini. Blood Cancer Journal, 2016, 6, e411-e411.	6.2	20
87	LFQProfiler and RNPxl: Open-Source Tools for Label-Free Quantification and Protein–RNA Cross-Linking Integrated into Proteome Discoverer. Journal of Proteome Research, 2016, 15, 3441-3448.	3.7	29
88	OpenMS: a flexible open-source software platform for mass spectrometry data analysis. Nature Methods, 2016, 13, 741-748.	19.0	537
89	Distinct transcriptional changes in non-small cell lung cancer patients associated with multi-antigenic RNActive® CV9201 immunotherapy. OncoImmunology, 2016, 5, e1249560.	4.6	18
90	Mass-Spectrometry-Based Proteomics Reveals Organ-Specific Expression Patterns To Be Used as Forensic Evidence. Journal of Proteome Research, 2016, 15, 182-192.	3.7	19

#	Article	IF	Citations
91	Recognizing millions of consistently unidentified spectra across hundreds of shotgun proteomics datasets. Nature Methods, 2016, 13, 651-656.	19.0	147
92	Improving global feature detectabilities through scan range splitting for untargeted metabolomics by high-performance liquid chromatography-Orbitrap mass spectrometry. Analytica Chimica Acta, 2016, 930, 13-22.	5.4	18
93	From the desktop to the grid: scalable bioinformatics via workflow conversion. BMC Bioinformatics, 2016, 17, 127.	2.6	12
94	Designing string-of-beads vaccines with optimal spacers. Genome Medicine, 2016, 8, 9.	8.2	41
95	Testing and Validation of Computational Methods for Mass Spectrometry. Journal of Proteome Research, 2016, 15, 809-814.	3.7	34
96	BALL-SNPgp—from genetic variants toward computational diagnostics. Bioinformatics, 2016, 32, 1888-1890.	4.1	0
97	FRED 2: an immunoinformatics framework for Python. Bioinformatics, 2016, 32, 2044-2046.	4.1	32
98	Challenges in Large-Scale Computational Mass Spectrometry and Multiomics. Journal of Proteome Research, 2016, 15, 681-682.	3.7	0
99	Learning from Heterogeneous Data Sources: An Application in Spatial Proteomics. PLoS Computational Biology, 2016, 12, e1004920.	3.2	47
100	Structural and Functional Characterization of the Bacterial Type III Secretion Export Apparatus. PLoS Pathogens, 2016, 12, e1006071.	4.7	66
101	Abstract A113: iVacALL: A personalized peptide-vaccination design platform for pediatric acute lymphoblastic leukemia patients based on patient-individual tumor-specific variants. , 2016, , .		0
102	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
103	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.	1.4	0
104	Copper oxide nanoparticle toxicity profiling using untargeted metabolomics. Particle and Fibre Toxicology, 2015, 13, 49.	6.2	65
105	The antigenic landscape of multiple myeloma: mass spectrometry (re)defines targets for T-cell—based immunotherapy. Blood, 2015, 126, 1203-1213.	1.4	103
106	Protein (multi-)location prediction: utilizing interdependencies via a generative model. Bioinformatics, 2015, 31, i365-i374.	4.1	21
107	Immunoinformatics and epitope prediction in the age of genomic medicine. Genome Medicine, 2015, 7, 119.	8.2	178
108	Intuitive Web-Based Experimental Design for High-Throughput Biomedical Data. BioMed Research International, 2015, 2015, 1-8.	1.9	3

#	Article	IF	Citations
109	Plants Release Precursors of Histone Deacetylase Inhibitors to Suppress Growth of Competitors. Plant Cell, 2015, 27, 3175-3189.	6.6	86
110	Dithiothreitol (DTT) Acts as a Specific, UV-inducible Cross-linker in Elucidation of Protein–RNA Interactions*. Molecular and Cellular Proteomics, 2015, 14, 3196-3210.	3.8	10
111	WIPI proteins: essential PtdIns3*P* effectors at the nascent autophagosome. Journal of Cell Science, 2015, 128, 207-17.	2.0	214
112	Workflows for automated downstream data analysis and visualization in large‐scale computational mass spectrometry. Proteomics, 2015, 15, 1443-1447.	2.2	32
113	Fluorescence-based imaging of autophagy progression by human WIPI protein detection. Methods, 2015, 75, 69-78.	3.8	17
114	Network-based interactive navigation and analysis of large biological datasets. IT - Information Technology, 2015, 57, 37-48.	0.9	0
115	Retention Time Prediction Improves Identification in Nontargeted Lipidomics Approaches. Analytical Chemistry, 2015, 87, 7698-7704.	6.5	80
116	Analysis of protein–RNA interactions in CRISPR proteins and effector complexes by UV-induced cross-linking and mass spectrometry. Methods, 2015, 89, 138-148.	3.8	25
117	EpiToolKit—a web-based workbench for vaccine design. Bioinformatics, 2015, 31, 2211-2213.	4.1	32
118	PIA: An Intuitive Protein Inference Engine with a Web-Based User Interface. Journal of Proteome Research, 2015, 14, 2988-2997.	3.7	69
119	Managing Expectations When Publishing Tools and Methods for Computational Proteomics. Journal of Proteome Research, 2015, 14, 2002-2004.	3.7	5
120	DNA-binding proteins from marine bacteria expand the known sequence diversity of TALE-like repeats. Nucleic Acids Research, 2015, 43, gkv1053.	14.5	23
121	Nephron Toxicity Profiling via Untargeted Metabolome Analysis Employing a High Performance Liquid Chromatography-Mass Spectrometry-based Experimental and Computational Pipeline. Journal of Biological Chemistry, 2015, 290, 19121-19132.	3.4	10
122	Dissecting neural differentiation regulatory networks through epigenetic footprinting. Nature, 2015, 518, 355-359.	27.8	172
123	MetaProSIP: Automated Inference of Stable Isotope Incorporation Rates in Proteins for Functional Metaproteomics. Journal of Proteome Research, 2015, 14, 619-627.	3.7	64
124	ballaxy: web services for structural bioinformatics. Bioinformatics, 2015, 31, 121-122.	4.1	10
125	Interplay Between the Immune System and Colorectal Carcinoma - Towards Tumor-Specific Peptide-Based Vaccination for Any HLA-Type. Blood, 2015, 126, 1027-1027.	1.4	0
126	BiNA: A Visual Analytics Tool for Biological Network Data. PLoS ONE, 2014, 9, e87397.	2.5	31

#	Article	IF	Citations
127	OptiType: precision HLA typing from next-generation sequencing data. Bioinformatics, 2014, 30, 3310-3316.	4.1	566
128	Performance Studies on Distributed Virtual Screening. BioMed Research International, 2014, 2014, 1-7.	1.9	8
129	qcML: An Exchange Format for Quality Control Metrics from Mass Spectrometry Experiments. Molecular and Cellular Proteomics, 2014, 13, 1905-1913.	3.8	42
130	The mzTab Data Exchange Format: Communicating Mass-spectrometry-based Proteomics and Metabolomics Experimental Results to a Wider Audience. Molecular and Cellular Proteomics, 2014, 13, 2765-2775.	3.8	130
131	Rebuilding KEGG Maps: Algorithms and Benefits. , 2014, , .		1
132	In melanoma, <scp>H</scp>ippo signaling is affected by copy number alterations and <scp>YAP</scp>1 overexpression impairs patient survival. Pigment Cell and Melanoma Research, 2014, 27, 671-673.	3.3	28
133	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.	2.6	35
134	Blocked Inverted Indices for Exact Clustering of Large Chemical Spaces. Journal of Chemical Information and Modeling, 2014, 54, 2395-2401.	5.4	9
135	Photo-cross-linking and high-resolution mass spectrometry for assignment of RNA-binding sites in RNA-binding proteins. Nature Methods, 2014, 11, 1064-1070.	19.0	218
136	The MoSGrid Science Gateway â€" A Complete Solution for Molecular Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2232-2245.	5.3	58
137	Time-resolved characterization of cAMP/PKA-dependent signaling reveals that platelet inhibition is a concerted process involving multiple signaling pathways. Blood, 2014, 123, e1-e10.	1.4	80
138	Activation of lymphoma-associated MyD88 mutations via allostery-induced TIR-domain oligomerization. Blood, 2014, 124, 3896-3904.	1.4	69
139	Automated Label-free Quantification of Metabolites from Liquid Chromatographyâ€"Mass Spectrometry Data. Molecular and Cellular Proteomics, 2014, 13, 348-359.	3.8	74
140	Clinical and non-targeted metabolomic profiling of homozygous carriers of Transcription Factor 7-like 2 variant rs7903146. Scientific Reports, 2014, 4, 5296.	3.3	17
141	Sequence co-evolution gives 3D contacts and structures of protein complexes. ELife, 2014, 3, .	6.0	452
142	Novel Visual Metaphors for Multivariate Networks. Lecture Notes in Computer Science, 2014, , 127-150.	1.3	3
143	Charting a dynamic DNA methylation landscape of the human genome. Nature, 2013, 500, 477-481.	27.8	1,168
144	Virtual screening and experimental validation reveal novel small-molecule inhibitors of 14-3-3 proteinâ€"protein interactions. Chemical Communications, 2013, 49, 8468.	4.1	40

#	Article	IF	Citations
145	An Automated Pipeline for High-Throughput Label-Free Quantitative Proteomics. Journal of Proteome Research, 2013, 12, 1628-1644.	3.7	146
146	Tools for Label-free Peptide Quantification. Molecular and Cellular Proteomics, 2013, 12, 549-556.	3.8	198
147	PTMeta: Increasing identification rates of modified peptides using modification prescanning and meta‐analysis. Proteomics, 2013, 13, 1042-1051.	2.2	5
148	Computational proteomics pitfalls and challenges: HavanaBioinfo 2012 Workshop report. Journal of Proteomics, 2013, 87, 134-138.	2.4	19
149	Transcriptional and Epigenetic Dynamics during Specification of Human Embryonic Stem Cells. Cell, 2013, 153, 1149-1163.	28.9	419
150	Interplay of pH and Binding of Multivalent Metal Ions: Charge Inversion and Reentrant Condensation in Protein Solutions. Journal of Physical Chemistry B, 2013, 117, 5777-5787.	2.6	97
151	The mzQuantML Data Standard for Mass Spectrometry–based Quantitative Studies in Proteomics. Molecular and Cellular Proteomics, 2013, 12, 2332-2340.	3.8	66
152	Elucidating the evolutionary conserved DNA-binding specificities of WRKY transcription factors by molecular dynamics and in vitro binding assays. Nucleic Acids Research, 2013, 41, 9764-9778.	14.5	161
153	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.	1.5	4
154	A Statistical Comparison of SimTandem with State-of-the-Art Peptide Identification Tools. Advances in Intelligent Systems and Computing, 2013, , 101-109.	0.6	1
155	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.	1.5	1
156	miHA-match. , 2012, , .		0
157	The mzIdentML Data Standard for Mass Spectrometry-Based Proteomics Results. Molecular and Cellular Proteomics, 2012, 11, M111.014381-1-M111.014381-10.	3.8	175
158	A Single Sign-On Infrastructure for Science Gateways on a Use Case for Structural Bioinformatics. Journal of Grid Computing, 2012, 10, 769-790.	3.9	39
159	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.	2.3	3
160	The bifunctional role of aconitase in <i><scp>S</scp>treptomyces viridochromogenes</i><scp>T</scp>Ã¼494. Environmental Microbiology, 2012, 14, 3203-3219.	3.8	13
161	miHA-Match: Computational detection of tissue-specific minor histocompatibility antigens. Journal of Immunological Methods, 2012, 386, 94-100.	1.4	7
162	In silico design of targeted SRM-based experiments. BMC Bioinformatics, 2012, 13, S8.	2.6	9

#	Article	IF	Citations
163	No Longer Confidential: Estimating the Confidence of Individual Regression Predictions. PLoS ONE, 2012, 7, e48723.	2.5	16
164	TOPPAS: A Graphical Workflow Editor for the Analysis of High-Throughput Proteomics Data. Journal of Proteome Research, 2012, 11, 3914-3920.	3.7	50
165	Covalent attachment of pyridoxal-phosphate derivatives to 14-3-3 proteins. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, E1051-3; author reply E1054.	7.1	18
166	Displacement chromatography as first separating step in online two-dimensional liquid chromatography coupled to mass spectrometry analysis of a complex protein sampleâ€"The proteome of neutrophils. Journal of Chromatography A, 2012, 1232, 288-294.	3.7	16
167	CADDSuite â€" a workflow-enabled suite of open-source tools for drug discovery. Journal of Cheminformatics, 2012, 4, .	6.1	8
168	Binding Pocket Optimization by Computational Protein Design. PLoS ONE, 2012, 7, e52505.	2.5	39
169	Workflow-enhanced conformational analysis of guanidine zinc complexes via a science gateway. Studies in Health Technology and Informatics, 2012, 175, 142-51.	0.3	2
170	Probabilistic Consensus Scoring Improves Tandem Mass Spectrometry Peptide Identification. Journal of Proteome Research, 2011, 10, 3332-3343.	3.7	45
171	OpenMS and TOPP: Open Source Software for LC-MS Data Analysis. Methods in Molecular Biology, 2011, 696, 353-367.	0.9	68
172	Bioinformatics for Qualitative and Quantitative Proteomics. Methods in Molecular Biology, 2011, 719, 331-349.	0.9	4
173	Universal peptide vaccines â€" Optimal peptide vaccine design based on viral sequence conservation. Vaccine, 2011, 29, 8745-8753.	3.8	35
174	No evidence of viral genomes in wholeâ€"transcriptome sequencing of three melanoma metastases. Experimental Dermatology, 2011, 20, 766-768.	2.9	4
175	Machine learning competition in immunology â€" Prediction of HLA class I binding peptides. Journal of Immunological Methods, 2011, 374, 1-4.	1.4	53
176	Molecular simulation grid. Journal of Cheminformatics, 2011, 3, .	6.1	0
177	MoSGrid â€" a molecular simulation grid as a new tool in computational chemistry, biology and material science. Journal of Cheminformatics, 2011, 3, .	6.1	1
178	A framework and workflow system for virtual screening and molecular docking. Journal of Cheminformatics, 2011, 3, .	6.1	0
179	POPISK: T-cell reactivity prediction using support vector machines and string kernels. BMC Bioinformatics, 2011, 12, 446.	2.6	79
180	T-cell epitope prediction based on self-tolerance. , 2011, , .		5

#	Article	IF	Citations
181	NRPSpredictor2—a web server for predicting NRPS adenylation domain specificity. Nucleic Acids Research, 2011, 39, W362-W367.	14.5	559
182	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.	2.3	7
183	BALL - biochemical algorithms library 1.3. BMC Bioinformatics, 2010, 11, 531.	2.6	62
184	Exploiting physico-chemical properties in string kernels. BMC Bioinformatics, 2010, 11, S7.	2.6	17
185	The role of phosphorylatable serine residues in the DNA-binding domain of Arabidopsis bZIP transcription factors. European Journal of Cell Biology, 2010, 89, 175-183.	3.6	42
186	Improved particle—packed HPLC/MS microchips for proteomic analysis. Journal of Separation Science, 2010, 33, 3283-3291.	2.5	7
187	Application of displacement chromatography for the proteome analysis of a human plasma protein fraction. Journal of Chromatography A, 2010, 1217, 3321-3329.	3.7	22
188	Universality of protein reentrant condensation in solution induced by multivalent metal ions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3450-3457.	2.6	106
189	Visualization of omics data for systems biology. Nature Methods, 2010, 7, S56-S68.	19.0	548
190	YLoc—an interpretable web server for predicting subcellular localization. Nucleic Acids Research, 2010, 38, W497-W502.	14.5	263
191	TOPP goes Rapid The OpenMS Proteomics Pipeline in a Grid-Enabled Web Portal. , 2010, , .		0
192	Combining Structure and Sequence Information Allows Automated Prediction of Substrate Specificities within Enzyme Families. PLoS Computational Biology, 2010, 6, e1000636.	3.2	36
193	Optimal de novo Design of MRM Experiments for Rapid Assay Development in Targeted Proteomics. Journal of Proteome Research, 2010, 9, 2696-2704.	3.7	40
194	OpenMS and TOPP: Open Source Software for LC-MS Data Analysis. Methods in Molecular Biology, 2010, 604, 201-211.	0.9	27
195	Going from where to why—interpretable prediction of protein subcellular localization. Bioinformatics, 2010, 26, 1232-1238.	4.1	133
196	Novel Machine Learning Methods for MHC Class I Binding Prediction. Lecture Notes in Computer Science, 2010, , 98-109.	1.3	30
197	A novel algorithm for detecting differentially regulated paths based on gene set enrichment analysis. Bioinformatics, 2009, 25, 2787-2794.	4.1	51
198	KIRMES: kernel-based identification of regulatory modules in euchromatic sequences. Bioinformatics, 2009, 25, 2126-2133.	4.1	21

#	Article	IF	Citations
199	FREDâ€"a framework for T-cell epitope detection. Bioinformatics, 2009, 25, 2758-2759.	4.1	20
200	OptiTope--a web server for the selection of an optimal set of peptides for epitope-based vaccines. Nucleic Acids Research, 2009, 37, W617-W622.	14.5	32
201	MultiLoc2: integrating phylogeny and Gene Ontology terms improves subcellular protein localization prediction. BMC Bioinformatics, 2009, 10, 274.	2.6	264
202	Modeling metabolic networks in C. glutamicum: a comparison of rate laws in combination with various parameter optimization strategies. BMC Systems Biology, 2009, 3, 5.	3.0	59
203	*De novo* peptide sequencing by tandem MS using complementary CID and electron transfer dissociation. Electrophoresis, 2009, 30, 3736-3747.	2.4	53
204	Automated scaffold selection for enzyme design. Proteins: Structure, Function and Bioinformatics, 2009, 77, 74-83.	2.6	45
205	Prediction of dual protein targeting to plant organelles. New Phytologist, 2009, 183, 224-236.	7.3	73
206	Improving Peptide Identification in Proteome Analysis by a Two-Dimensional Retention Time Filtering Approach. Journal of Proteome Research, 2009, 8, 4109-4115.	3.7	36
207	SherLoc2: A High-Accuracy Hybrid Method for Predicting Subcellular Localization of Proteins. Journal of Proteome Research, 2009, 8, 5363-5366.	3.7	122
208	TOPPView: An Open-Source Viewer for Mass Spectrometry Data. Journal of Proteome Research, 2009, 8, 3760-3763.	3.7	74
209	Towards *in silico* design of epitope-based vaccines. Expert Opinion on Drug Discovery, 2009, 4, 1047-1060.	5.0	18
210	Simultaneous alignment of short reads against multiple genomes. Genome Biology, 2009, 10, R98.	9.6	215
211	Integer Linear Programming in Computational Biology. Lecture Notes in Computer Science, 2009, , 199-218.	1.3	5
212	Implications for selectivity of 3,4-diarylquinolinones as p38Î±MAP kinase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 1431-1435.	2.2	48
213	OpenMS â€" An open-source software framework for mass spectrometry. BMC Bioinformatics, 2008, 9, 163.	2.6	556
214	LC-MSsim â€" a simulation software for liquid chromatography mass spectrometry data. BMC Bioinformatics, 2008, 9, 423.	2.6	42
215	Peak intensity prediction in MALDI-TOF mass spectrometry: A machine learning study to support quantitative proteomics. BMC Bioinformatics, 2008, 9, 443.	2.6	30
216	GeneTrailExpress: a web-based pipeline for the statistical evaluation of microarray experiments. BMC Bioinformatics, 2008, 9, 552.	2.6	69

#	Article	IF	Citations
217	BALLDock/SLICK: A New Method for Protein-Carbohydrate Docking. Journal of Chemical Information and Modeling, 2008, 48, 1616-1625.	5.4	52
218	EpiToolKitâ€"a web server for computational immunomics. Nucleic Acids Research, 2008, 36, W519-W522.	14.5	21
219	Using Atom Mapping Rules for an Improved Detection of Relevant Routes in Weighted Metabolic Networks. Journal of Computational Biology, 2008, 15, 565-576.	1.6	41
220	MetaRoute: fast search for relevant metabolic routes for interactive network navigation and visualization. Bioinformatics, 2008, 24, 2108-2109.	4.1	68
221	A Mathematical Framework for the Selection of an Optimal Set of Peptides for Epitope-Based Vaccines. PLoS Computational Biology, 2008, 4, e1000246.	3.2	32
222	Reentrant Condensation of Proteins in Solution Induced by Multivalent Counterions. Physical Review Letters, 2008, 101, 148101.	7.8	184
223	Multiple Instance Learning Allows MHC Class II Epitope Predictions Across Alleles. Lecture Notes in Computer Science, 2008, , 210-221.	1.3	19
224	A statistical learning approach to the modeling of chromatographic retention of oligonucleotides incorporating sequence and secondary structure data. Nucleic Acids Research, 2007, 35, 4195-4202.	14.5	23
225	Electrostatic potentials of proteins in water: a structured continuum approach. Bioinformatics, 2007, 23, e99-e103.	4.1	41
226	SherLoc: high-accuracy prediction of protein subcellular localization by integrating text and protein sequence data. Bioinformatics, 2007, 23, 1410-1417.	4.1	113
227	BNDB â€" The Biochemical Network Database. BMC Bioinformatics, 2007, 8, 367.	2.6	36
228	Statistical learning of peptide retention behavior in chromatographic separations: a new kernel-based approach for computational proteomics. BMC Bioinformatics, 2007, 8, 468.	2.6	70
229	TOPP--the OpenMS proteomics pipeline. Bioinformatics, 2007, 23, e191-e197.	4.1	249
230	Profile and Molecular Modeling of 3-(Indole-3-yl)-4-(3,4,5-trimethoxyphenyl)-1H-pyrrole-2,5dione (1) as a Highly Selective VEGF-R2/3 Inhibitor. Journal of Medicinal Chemistry, 2006, 49, 7549-7553.	6.4	29
231	A Fully Computational Model for Predicting Percutaneous Drug Absorption. Journal of Chemical Information and Modeling, 2006, 46, 424-429.	5.4	46
232	SLICK â€" Scoring and Energy Functions for Proteinâ€"Carbohydrate Interactions. Journal of Chemical Information and Modeling, 2006, 46, 1635-1642.	5.4	40
233	Absolute Myoglobin Quantitation in Serum by Combining Two-Dimensional Liquid Chromatographyâ€"Electrospray Ionization Mass Spectrometry and Novel Data Analysis Algorithms. Journal of Proteome Research, 2006, 5, 414-421.	3.7	77
234	Development of a fluorescence-based assay for screening of modulators of human Organic Anion Transporter 1B3 (OATP1B3). European Journal of Pharmaceutics and Biopharmaceutics, 2006, 62, 39-43.	4.3	38

#	Article	IF	Citations
235	BN++ â€" A Biological Information System. Journal of Integrative Bioinformatics, 2006, 3, 148-161.	1.5	17
236	MultiLoc: prediction of protein subcellular localization using N-terminal targeting sequences, sequence motifs and amino acid composition. Bioinformatics, 2006, 22, 1158-1165.	4.1	290
237	Structureâ€"Activity Relationships in Chromatography: Retention Prediction of Oligonucleotides with Support Vector Regression. Angewandte Chemie - International Edition, 2006, 45, 7009-7012.	13.8	21
238	SVMHC: a server for prediction of MHC-binding peptides. Nucleic Acids Research, 2006, 34, W194-W197.	14.5	79
239	BALLView: a tool for research and education in molecular modeling. Bioinformatics, 2006, 22, 365-366.	4.1	53
240	High-accuracy peak picking of proteomics data using wavelet techniques. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2006, , 243-54.	0.7	22
241	SIGNIFICANTLY IMPROVED PREDICTION OF SUBCELLULAR LOCALIZATION BY INTEGRATING TEXT AND PROTEIN SEQUENCE DATA. , 2005, , .		11
242	HIGH-ACCURACY PEAK PICKING OF PROTEOMICS DATA USING WAVELET TECHNIQUES. , 2005, , .		33
243	Integrated modeling of the major events in the MHC class I antigen processing pathway. Protein Science, 2005, 14, 2132-2140.	7.6	76
244	SNEP: SNP-derived Epitope Prediction program for minor H antigens. Immunogenetics, 2005, 57, 816-820.	2.4	26
245	BALLView: An object-oriented molecular visualization and modeling framework. Journal of Computer-Aided Molecular Design, 2005, 19, 791-800.	2.9	40
246	Specificity prediction of adenylation domains in nonribosomal peptide synthetases (NRPS) using transductive support vector machines (TSVMs). Nucleic Acids Research, 2005, 33, 5799-5808.	14.5	388
247	Analysis of MHC-Peptide Binding Using Amino Acid Property-Based Decision Rules. Lecture Notes in Computer Science, 2005, , 446-453.	1.3	2
248	Algorithms for the Automated Absolute Quantification of Diagnostic Markers in Complex Proteomics Samples. Lecture Notes in Computer Science, 2005, , 151-162.	1.3	4
249	Novel Formulation of Nonlocal Electrostatics. Physical Review Letters, 2004, 93, 108104.	7.8	83
250	Comparative immunopeptidomics of humans and their pathogens. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 13268-13272.	7.1	38
251	Integrative analysis of cancerâ€related data using CAP. FASEB Journal, 2004, 18, 1465-1467.	0.5	9
252	Computational modeling of the sugarâ€"lectin interaction. Advanced Drug Delivery Reviews, 2004, 56, 437-457.	13.7	43

#	Article	IF	Citations
253	From sequence to structure and back again: approaches for predicting protein-DNA binding. Proteome Science, 2004, 2, 3.	1.7	21
254	Epitope prediction algorithms for peptide-based vaccine design. Proceedings, 2003, 2, 17-26.	0.1	16
255	A Combinatorial Approach to Protein Docking with Flexible Side Chains. Journal of Computational Biology, 2002, 9, 597-612.	1.6	54
256	Lectin-sugar interaction. FEBS Journal, 2002, 269, 1518-1524.	0.2	26
257	Structure prediction of protein complexes by an NMR-based protein docking algorithm. Journal of Biomolecular NMR, 2001, 20, 15-21.	2.8	16
258	BALL: Biochemical Algorithms Library. Lecture Notes in Computer Science, 1999, , 330-344.	1.3	5
259	Modeling Protein-Protein and Protein-DNA Docking. , 0, , 601-650.		2