Sebastian BÃ¶cker

List of Publications by Year
in descending order

132	7,251	71102 41	66911 78
papers	citations	h-index	g-index

152	152	152	6445
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High-confidence structural annotation of metabolites absent from spectral libraries. Nature Biotechnology, 2022, 40, 411-421.	17.5	100
2	Current state-of-the-art of separation methods used in LC-MS based metabolomics and lipidomics. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2022, 1188, 123069.	2.3	44
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	MSNovelist: de novo structure generation from mass spectra. Nature Methods, 2022, 19, 865-870.	19.0	49
5	Mass Difference Matching Unfolds Hidden Molecular Structures of Dissolved Organic Matter. Environmental Science & Technology, 2022, 56, 11027-11040.	10.0	5
6	Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. Nature Biotechnology, 2021, 39, 462-471.	17.5	317
7	Studying Charge Migration Fragmentation of Sodiated Precursor Ions in Collision-Induced Dissociation at the Library Scale. Journal of the American Society for Mass Spectrometry, 2021, 32, 180-186.	2.8	4
8	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. Nature Chemical Biology, 2021, 17, 146-151.	8.0	73
9	Ion identity molecular networking for mass spectrometry-based metabolomics in the GNPS environment. Nature Communications, 2021, 12, 3832.	12.8	119
10	Database-independent molecular formula annotation using Gibbs sampling through ZODIAC. Nature Machine Intelligence, 2020, 2, 629-641.	16.0	103
11	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	19.0	650
12	Current status of retention time prediction in metabolite identification. Journal of Separation Science, 2020, 43, 1746-1754.	2.5	71
13	De Novo Molecular Formula Annotation and Structure Elucidation Using SIRIUS 4. Methods in Molecular Biology, 2020, 2104, 185-207.	0.9	11
14	Drosophila melanogaster chemical ecology revisited: 2-D distribution maps of sex pheromones on whole virgin and mated flies by mass spectrometry imaging. BMC Zoology, 2020, 5, .	1.0	2
15	SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. Nature Methods, 2019, 16, 299-302.	19.0	822
16	Secondary ion mass spectrometry imaging and multivariate data analysis reveal coâ€aggregation patterns of Populus trichocarpa leaf surface compounds on a micrometer scale. Plant Journal, 2018, 93, 193-206.	5.7	22
17	Expanding the Use of Spectral Libraries in Proteomics. Journal of Proteome Research, 2018, 17, 4051-4060.	3.7	47
18	Liquid-chromatography retention order prediction for metabolite identification. Bioinformatics, 2018, 34, i875-i883.	4.1	52

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19	Bayesian networks for mass spectrometric metabolite identification via molecular fingerprints. Bioinformatics, 2018, 34, i333-i340.	4.1	36
20	Mining molecular structure databases: Identification of small molecules based on fragmentation mass spectrometry data. Mass Spectrometry Reviews, 2017, 36, 624-633.	5.4	75
21	Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples. RSC Advances, 2017, 7, 9045-9050.	3.6	28
22	Searching molecular structure databases using tandem MS data: are we there yet?. Current Opinion in Chemical Biology, 2017, 36, 1-6.	6.1	53
23	Bad Clade Deletion Supertrees: A Fast and Accurate Supertree Algorithm. Molecular Biology and Evolution, 2017, 34, 2408-2421.	8.9	10
24	LifeStyle-Specific-Islands (LiSSI): Integrated Bioinformatics Platform for Genomic Island Analysis. Journal of Integrative Bioinformatics, 2017, 14, .	1.5	1
25	Significance estimation for large scale metabolomics annotations by spectral matching. Nature Communications, 2017, 8, 1494.	12.8	128
26	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	6.1	122
27	Exploring the Limits of the Geometric Copolymerization Model. Polymers, 2017, 9, 101.	4.5	1
28	New Statistical Models for Copolymerization. Polymers, 2016, 8, 240.	4.5	5
29	Finding approximate gene clusters with Gecko 3. Nucleic Acids Research, 2016, 44, gkw843.	14.5	23
30	Predicting the Presence of Uncommon Elements in Unknown Biomolecules from Isotope Patterns. Analytical Chemistry, 2016, 88, 7556-7566.	6.5	26
31	Abundance correction for mass discrimination effects in polymer mass spectra. Rapid Communications in Mass Spectrometry, 2016, 30, 1233-1241.	1.5	5
32	Fast metabolite identification with Input Output Kernel Regression. Bioinformatics, 2016, 32, i28-i36.	4.1	57
33	Fragmentation trees reloaded. Journal of Cheminformatics, 2016, 8, 5.	6.1	138
34	Collecting reliable clades using the Greedy Strict Consensus Merger. PeerJ, 2016, 4, e2172.	2.0	5
35	Ten Times Eighteen. Journal of Information Processing, 2015, 23, 258-264.	0.4	0
36	COCONUTâ€"An Efficient Tool for Estimating Copolymer Compositions from Mass Spectra. Analytical Chemistry, 2015, 87, 5223-5231.	6.5	19

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37	Searching molecular structure databases with tandem mass spectra using CSI:FingerID. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12580-12585.	7.1	695
38	Correcting mass shifts: A lock mass-free recalibration procedure for mass spectrometry imaging data. Analytical and Bioanalytical Chemistry, 2015, 407, 7603-7613.	3.7	11
39	Fragmentation Trees Reloaded. Lecture Notes in Computer Science, 2015, , 65-79.	1.3	6
40	Speedy Colorful Subtrees. Lecture Notes in Computer Science, 2015, , 310-322.	1.3	5
41	Molecular Formula Identification Using Isotope Pattern Analysis and Calculation of Fragmentation Trees. Mass Spectrometry, 2014, 3, S0037-S0037.	0.6	20
42	Metabolite identification through multiple kernel learning on fragmentation trees. Bioinformatics, 2014, 30, i157-i164.	4.1	87
43	Gene Expansion Shapes Genome Architecture in the Human Pathogen Lichtheimia corymbifera: An Evolutionary Genomics Analysis in the Ancient Terrestrial Mucorales (Mucoromycotina). PLoS Genetics, 2014, 10, e1004496.	3.5	80
44	Mass spectrometry imaging of surface lipids on intact Drosophila melanogaster flies. Journal of Mass Spectrometry, 2014, 49, 223-232.	1.6	30
45	New kids on the block: novel informatics methods for natural product discovery. Natural Product Reports, 2014, 31, 807.	10.3	64
46	Munronia pinnata (Wall.) Theob.: Unveiling phytochemistry and dual inhibition of 5-lipoxygenase and microsomal prostaglandin E2 synthase (mPGES)-1. Journal of Ethnopharmacology, 2014, 151, 882-890.	4.1	7
47	Counting glycans revisited. Journal of Mathematical Biology, 2014, 69, 799-816.	1.9	1
48	Computational mass spectrometry for small-molecule fragmentation. TrAC - Trends in Analytical Chemistry, 2014, 53, 41-48.	11.4	86
49	Identifying gene clusters by discovering common intervals in indeterminate strings. BMC Genomics, 2014, 15, S2.	2.8	4
50	Computational mass spectrometry for small molecules. Journal of Cheminformatics, 2013, 5, 12.	6.1	122
51	FlipCut Supertrees: Towards Matrix Representation Accuracy in Polynomial Time. Algorithmica, 2013, 67, 142-160.	1.3	4
52	Statistics for approximate gene clusters. BMC Bioinformatics, 2013, 14, S14.	2.6	11
53	Finding Maximum Colorful Subtrees in Practice. Journal of Computational Biology, 2013, 20, 311-321.	1.6	16
54	Molecular Formula Identification with SIRIUS. Metabolites, 2013, 3, 506-516.	2.9	34

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55	Cluster Editing. Lecture Notes in Computer Science, 2013, , 33-44.	1.3	22
56	The Generalized Robinson-Foulds Metric. Lecture Notes in Computer Science, 2013, , 156-169.	1.3	14
57	Faster Mass Decomposition. Lecture Notes in Computer Science, 2013, , 45-58.	1.3	6
58	Fast alignment of fragmentation trees. Bioinformatics, 2012, 28, i265-i273.	4.1	14
59	Improved Fixed-Parameter Algorithms for Minimum-Flip Consensus Trees. ACM Transactions on Algorithms, 2012, 8, 1-17.	1.0	3
60	Identifying the Unknowns by Aligning Fragmentation Trees. Analytical Chemistry, 2012, 84, 3417-3426.	6.5	104
61	Comment on: â€œAn Efficient Method to Calculate the Aggregated Isotopic Distribution and Exact Center-Massesâ€•by JÃ¼rgen Claesen, Piotr Dittwald, Tomasz Burzykowski, Dirk Valkenborg, J. Am. Soc. Mass Spectrom. 2012, 23, 753â€“763. Journal of the American Society for Mass Spectrometry, 2012, 23, 1826-1827.	2.8	5
62	De novo analysis of electron impact mass spectra using fragmentation trees. Analytica Chimica Acta, 2012, 739, 67-76.	5.4	26
63	A golden ratio parameterized algorithm for Cluster Editing. Journal of Discrete Algorithms, 2012, 16, 79-89.	0.7	36
64	Determination of ¹⁵N-Incorporation into Plant Proteins and their Absolute Quantitation: A New Tool to Study Nitrogen Flux Dynamics and Protein Pool Sizes Elicited by Plantâ€“Herbivore Interactions. Journal of Proteome Research, 2012, 11, 4947-4960.	3.7	15
65	A note on the parameterized complexity of unordered maximum tree orientation. Discrete Applied Mathematics, 2012, 160, 1634-1638.	0.9	2
66	Finding Maximum Colorful Subtrees in Practice. Lecture Notes in Computer Science, 2012, , 213-223.	1.3	3
67	Determination of Glycan Structure from Tandem Mass Spectra. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2011, 8, 976-986.	3.0	19
68	Computing Fragmentation Trees from Tandem Mass Spectrometry Data. Analytical Chemistry, 2011, 83, 1243-1251.	6.5	134
69	Extension and Robustness of Transitivity Clustering for Proteinâ€“Protein Interaction Network Analysis. Internet Mathematics, 2011, 7, 255-273.	0.7	8
70	Polynomial Supertree Methods Revisited. Advances in Bioinformatics, 2011, 2011, 1-21.	5.7	7
71	Comprehensive cluster analysis with Transitivity Clustering. Nature Protocols, 2011, 6, 285-295.	12.0	47
72	Exact Algorithms for Cluster Editing: Evaluation and Experiments. Algorithmica, 2011, 60, 316-334.	1.3	71

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73	Combinatorics of aliphatic amino acids. Die Naturwissenschaften, 2011, 98, 79-86.	1.6	5
74	Swiftly Computing Center Strings. BMC Bioinformatics, 2011, 12, 106.	2.6	4
75	Analysis of different synthetic homopolymers by the use of a new calculation software for tandem mass spectra. Rapid Communications in Mass Spectrometry, 2011, 25, 1765-1778.	1.5	13
76	Even faster parameterized cluster deletion and cluster editing. Information Processing Letters, 2011, 111, 717-721.	0.6	31
77	Computing bond orders in molecule graphs. Theoretical Computer Science, 2011, 412, 1184-1195.	0.9	3
78	Automated bond order assignment as an optimization problem. Bioinformatics, 2011, 27, 619-625.	4.1	13
79	Computing Fragmentation Trees from Metabolite Multiple Mass Spectrometry Data. Journal of Computational Biology, 2011, 18, 1383-1397.	1.6	25
80	Computing Fragmentation Trees from Metabolite Multiple Mass Spectrometry Data. Lecture Notes in Computer Science, 2011, , 377-391.	1.3	2
81	A Golden Ratio Parameterized Algorithm for Cluster Editing. Lecture Notes in Computer Science, 2011, , 85-95.	1.3	4
82	FlipCut Supertrees: Towards Matrix Representation Accuracy in Polynomial Time. Lecture Notes in Computer Science, 2011, , 37-48.	1.3	1
83	Computational mass spectrometry for metabolomics: Identification of metabolites and small molecules. Analytical and Bioanalytical Chemistry, 2010, 398, 2779-2788.	3.7	159
84	Partitioning biological data with transitivity clustering. Nature Methods, 2010, 7, 419-420.	19.0	84
85	Exact ILP solutions for phylogenetic minimum flip problems. , 2010, , .		39
86	Swiftly Computing Center Strings. Lecture Notes in Computer Science, 2010, , 325-336.	1.3	11
87	Polynomial Supertree Methods Revisited. Lecture Notes in Computer Science, 2010, , 183-194.	1.3	2
88	Unbiased Transcriptional Comparisons of Generalist and Specialist Herbivores Feeding on Progressively Defenseless Nicotiana attenuata Plants. PLoS ONE, 2010, 5, e8735.	2.5	95
89	Computation of Median Gene Clusters. Journal of Computational Biology, 2009, 16, 1085-1099.	1.6	32
90	SIRIUS: decomposing isotope patterns for metabolite identification. Bioinformatics, 2009, 25, 218-224.	4.1	276

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91	On optimal comparability editing with applications to molecular diagnostics. BMC Bioinformatics, 2009, 10, S61.	2.6	5
92	De novo peptide sequencing by tandem MS using complementary CID and electron transfer dissociation. Electrophoresis, 2009, 30, 3736-3747.	2.4	53
93	Determination of Glycan Structure from Tandem Mass Spectra. Lecture Notes in Computer Science, 2009, , 258-267.	1.3	1
94	Computing Bond Types in Molecule Graphs. Lecture Notes in Computer Science, 2009, , 297-306.	1.3	2
95	Annotating Fragmentation Patterns. Lecture Notes in Computer Science, 2009, , 13-24.	1.3	9
96	A Faster Fixed-Parameter Approach to Drawing Binary Tanglegrams. Lecture Notes in Computer Science, 2009, , 38-49.	1.3	17
97	Inferring Peptide Composition from Molecular Formulas. Lecture Notes in Computer Science, 2009, , 277-286.	1.3	0
98	Peak intensity prediction in MALDI-TOF mass spectrometry: A machine learning study to support quantitative proteomics. BMC Bioinformatics, 2008, 9, 443.	2.6	30
99	Combinatorial Approaches for Mass Spectra Recalibration. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2008, 5, 91-100.	3.0	9
100	Towards de novo identification of metabolites by analyzing tandem mass spectra. Bioinformatics, 2008, 24, i49-i55.	4.1	110
101	D<scp>ecomp</scp>â€”from interpreting Mass Spectrometry peaks to solving the Money Changing Problem. Bioinformatics, 2008, 24, 591-593.	4.1	18
102	EPoS: a modular software framework for phylogenetic analysis. Bioinformatics, 2008, 24, 2399-2400.	4.1	41
103	Exact Algorithms for Cluster Editing: Evaluation and Experiments. , 2008, , 289-302.		8
104	Computation of Median Gene Clusters. Lecture Notes in Computer Science, 2008, , 331-345.	1.3	8
105	Going Weighted: Parameterized Algorithms for Cluster Editing. Lecture Notes in Computer Science, 2008, , 1-12.	1.3	8
106	Simulating multiplexed SNP discovery rates using base-specific cleavage and mass spectrometry. Bioinformatics, 2007, 23, e5-e11.	4.1	25
107	Mass spectra alignments and their significance. Journal of Discrete Algorithms, 2007, 5, 714-728.	0.7	5
108	SAMPI: Protein Identification with Mass Spectra Alignments. BMC Bioinformatics, 2007, 8, 102.	2.6	7

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109	A Fast and Simple Algorithm for the Money Changing Problem. Algorithmica, 2007, 48, 413-432.	1.3	57
110	A FIXED-PARAMETER APPROACH FOR WEIGHTED CLUSTER EDITING. , 2007, , .		2
111	EXACT AND HEURISTIC ALGORITHMS FOR WEIGHTED CLUSTER EDITING. , 2007, , .		43
112	Exact and heuristic algorithms for weighted cluster editing. Computational Systems Bioinformatics / Life Sciences Society Computational Systems Bioinformatics Conference, 2007, 6, 391-401.	0.4	13
113	Sequencing from Compomers: The Puzzle. Theory of Computing Systems, 2006, 39, 455-471.	1.1	1
114	Decomposing Metabolomic Isotope Patterns. Lecture Notes in Computer Science, 2006, , 12-23.	1.3	16
115	Markov Additive Chains and Applications to Fragment Statistics for Peptide Mass Fingerprinting. Lecture Notes in Computer Science, 2006, , 29-41.	1.3	2
116	Efficient mass decomposition. , 2005, , .		11
117	Mass Spectra Alignments and Their Significance. Lecture Notes in Computer Science, 2005, , 429-441.	1.3	3
118	Multiplexed discovery of sequence polymorphisms using base-specific cleavage and MALDI-TOF MS. Nucleic Acids Research, 2005, 33, e38-e38.	14.5	78
119	Novel Mass Spectrometry-Based Tool for Genotypic Identification of Mycobacteria. Journal of Clinical Microbiology, 2004, 42, 339-346.	3.9	89
120	Sequencing from Compomers: Using Mass Spectrometry for DNAde novoSequencing of 200+ nt. Journal of Computational Biology, 2004, 11, 1110-1134.	1.6	22
121	Unrooted Supertrees. Computational Biology, 2004, , 331-351.	0.2	1
122	SNP and mutation discovery using base-specific cleavage and MALDI-TOF mass spectrometry. Bioinformatics, 2003, 19, i44-i53.	4.1	42
123	High-Throughput MALDI-TOF Discovery of Genomic Sequence Polymorphisms. Genome Research, 2003, 14, 126-133.	5.5	114
124	RNase T1 mediated base-specific cleavage and MALDI-TOF MS for high-throughput comparative sequence analysis. Nucleic Acids Research, 2003, 31, 47e-47.	14.5	76
125	Base-specific fragmentation of amplified 16S rRNA genes analyzed by mass spectrometry: A tool for rapid bacterial identification. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 7039-7044.	7.1	122
126	Exponentially many supertrees. Applied Mathematics Letters, 2002, 15, 861-865.	2.7	3

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127	Patchworks. Advances in Mathematics, 2001, 157, 1-21.	1.1	8
128	A Note on Maximal Hierarchies. Advances in Mathematics, 2000, 151, 270-282.	1.1	5
129	Algorithmic Aspects of Tree Amalgamation. Journal of Algorithms, 2000, 37, 522-537.	0.9	33
130	Simple but Fundamental Limitations on Supertree and Consensus Tree Methods. Systematic Biology, 2000, 49, 363-368.	5.6	77
131	Patching upX-trees. Annals of Combinatorics, 1999, 3, 1-12.	0.6	15
132	Recovering Symbolically Dated, Rooted Trees from Symbolic Ultrametrics. Advances in Mathematics, 1998, 138, 105-125.	1.1	51