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	SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. Nature Methods, 2019, 16, 299-302.	19.0	822
2	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
3	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	19.0	650
4	Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. Nature Biotechnology, 2021, 39, 462-471.	17.5	317
5	SIRIUS: decomposing isotope patterns for metabolite identification. Bioinformatics, 2009, 25, 218-224.	4.1	276
6	Computational mass spectrometry for metabolomics: Identification of metabolites and small molecules. Analytical and Bioanalytical Chemistry, 2010, 398, 2779-2788.	3.7	159
7	Fragmentation trees reloaded. Journal of Cheminformatics, 2016, 8, 5.	6.1	138
8	Computing Fragmentation Trees from Tandem Mass Spectrometry Data. Analytical Chemistry, 2011, 83, 1243-1251.	6.5	134
9	Significance estimation for large scale metabolomics annotations by spectral matching. Nature Communications, 2017, 8, 1494.	12.8	128
10	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
11	Computational mass spectrometry for small molecules. Journal of Cheminformatics, 2013, 5, 12.	6.1	122
12	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	6.1	122
13	Ion identity molecular networking for mass spectrometry-based metabolomics in the GNPS environment. Nature Communications, 2021, 12, 3832.	12.8	119
14	High-Throughput MALDI-TOF Discovery of Genomic Sequence Polymorphisms. Genome Research, 2003, 14, 126-133.	5.5	114
15	Towards de novo identification of metabolites by analyzing tandem mass spectra. Bioinformatics, 2008, 24, i49-i55.	4.1	110
16	Identifying the Unknowns by Aligning Fragmentation Trees. Analytical Chemistry, 2012, 84, 3417-3426.	6.5	104
17	Database-independent molecular formula annotation using Gibbs sampling through ZODIAC. Nature Machine Intelligence, 2020, 2, 629-641.	16.0	103
18	High-confidence structural annotation of metabolites absent from spectral libraries. Nature Biotechnology, 2022, 40, 411-421.	17.5	100

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19	Unbiased Transcriptional Comparisons of Generalist and Specialist Herbivores Feeding on Progressively Defenseless Nicotiana attenuata Plants. PLoS ONE, 2010, 5, e8735.	2.5	95
20	Novel Mass Spectrometry-Based Tool for Genotypic Identification of Mycobacteria. Journal of Clinical Microbiology, 2004, 42, 339-346.	3.9	89
21	Metabolite identification through multiple kernel learning on fragmentation trees. Bioinformatics, 2014, 30, i157-i164.	4.1	87
22	Computational mass spectrometry for small-molecule fragmentation. TrAC - Trends in Analytical Chemistry, 2014, 53, 41-48.	11.4	86
23	Partitioning biological data with transitivity clustering. Nature Methods, 2010, 7, 419-420.	19.0	84
24	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
25	Multiplexed discovery of sequence polymorphisms using base-specific cleavage and MALDI-TOF MS. Nucleic Acids Research, 2005, 33, e38-e38.	14.5	78
26	Simple but Fundamental Limitations on Supertree and Consensus Tree Methods. Systematic Biology, 2000, 49, 363-368.	5.6	77
27	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
28	Mining molecular structure databases: Identification of small molecules based on fragmentation mass spectrometry data. Mass Spectrometry Reviews, 2017, 36, 624-633.	5.4	75
29	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. Nature Chemical Biology, 2021, 17, 146-151.	8.0	73
30	Exact Algorithms for Cluster Editing: Evaluation and Experiments. Algorithmica, 2011, 60, 316-334.	1.3	71
31	Current status of retention time prediction in metabolite identification. Journal of Separation Science, 2020, 43, 1746-1754.	2.5	71
32	New kids on the block: novel informatics methods for natural product discovery. Natural Product Reports, 2014, 31, 807.	10.3	64
33	A Fast and Simple Algorithm for the Money Changing Problem. Algorithmica, 2007, 48, 413-432.	1.3	57
34	Fast metabolite identification with Input Output Kernel Regression. Bioinformatics, 2016, 32, i28-i36.	4.1	57
35	De novo peptide sequencing by tandem MS using complementary CID and electron transfer dissociation. Electrophoresis, 2009, 30, 3736-3747.	2.4	53
36	Searching molecular structure databases using tandem MS data: are we there yet?. Current Opinion in Chemical Biology, 2017, 36, 1-6.	6.1	53

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37	Liquid-chromatography retention order prediction for metabolite identification. Bioinformatics, 2018, 34, i875-i883.	4.1	52
38	Recovering Symbolically Dated, Rooted Trees from Symbolic Ultrametrics. Advances in Mathematics, 1998, 138, 105-125.	1.1	51
39	MSNovelist: de novo structure generation from mass spectra. Nature Methods, 2022, 19, 865-870.	19.0	49
40	Comprehensive cluster analysis with Transitivity Clustering. Nature Protocols, 2011, 6, 285-295.	12.0	47
41	Expanding the Use of Spectral Libraries in Proteomics. Journal of Proteome Research, 2018, 17, 4051-4060.	3.7	47
42	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
43	EXACT AND HEURISTIC ALGORITHMS FOR WEIGHTED CLUSTER EDITING. , 2007, , .		43
44	SNP and mutation discovery using base-specific cleavage and MALDI-TOF mass spectrometry. Bioinformatics, 2003, 19, i44-i53.	4.1	42
45	EPoS: a modular software framework for phylogenetic analysis. Bioinformatics, 2008, 24, 2399-2400.	4.1	41
46	Exact ILP solutions for phylogenetic minimum flip problems. , 2010, , .		39
47	A golden ratio parameterized algorithm for Cluster Editing. Journal of Discrete Algorithms, 2012, 16, 79-89.	0.7	36
48	Bayesian networks for mass spectrometric metabolite identification via molecular fingerprints. Bioinformatics, 2018, 34, i333-i340.	4.1	36
49	Molecular Formula Identification with SIRIUS. Metabolites, 2013, 3, 506-516.	2.9	34
50	Algorithmic Aspects of Tree Amalgamation. Journal of Algorithms, 2000, 37, 522-537.	0.9	33
51	Computation of Median Gene Clusters. Journal of Computational Biology, 2009, 16, 1085-1099.	1.6	32
52	Even faster parameterized cluster deletion and cluster editing. Information Processing Letters, 2011, 111, 717-721.	0.6	31
53	Peak intensity prediction in MALDI-TOF mass spectrometry: A machine learning study to support quantitative proteomics. BMC Bioinformatics, 2008, 9, 443.	2.6	30
54	Mass spectrometry imaging of surface lipids on intact Drosophila melanogaster flies. Journal of Mass Spectrometry, 2014, 49, 223-232.	1.6	30

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55	Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples. RSC Advances, 2017, 7, 9045-9050.	3.6	28
56	De novo analysis of electron impact mass spectra using fragmentation trees. Analytica Chimica Acta, 2012, 739, 67-76.	5.4	26
57	Predicting the Presence of Uncommon Elements in Unknown Biomolecules from Isotope Patterns. Analytical Chemistry, 2016, 88, 7556-7566.	6.5	26
58	Simulating multiplexed SNP discovery rates using base-specific cleavage and mass spectrometry. Bioinformatics, 2007, 23, e5-e11.	4.1	25
59	Computing Fragmentation Trees from Metabolite Multiple Mass Spectrometry Data. Journal of Computational Biology, 2011, 18, 1383-1397.	1.6	25
60	Finding approximate gene clusters with Gecko 3. Nucleic Acids Research, 2016, 44, gkw843.	14.5	23
61	Sequencing from Compomers: Using Mass Spectrometry for DNAde novoSequencing of 200+ nt. Journal of Computational Biology, 2004, 11, 1110-1134.	1.6	22
62	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
63	Cluster Editing. Lecture Notes in Computer Science, 2013, , 33-44.	1.3	22
64	Molecular Formula Identification Using Isotope Pattern Analysis and Calculation of Fragmentation Trees. Mass Spectrometry, 2014, 3, S0037-S0037.	0.6	20
65	Determination of Glycan Structure from Tandem Mass Spectra. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2011, 8, 976-986.	3.0	19
66	COCONUTâ€"An Efficient Tool for Estimating Copolymer Compositions from Mass Spectra. Analytical Chemistry, 2015, 87, 5223-5231.	6.5	19
67	D<scp>ecomp</scp>â€"from interpreting Mass Spectrometry peaks to solving the Money Changing Problem. Bioinformatics, 2008, 24, 591-593.	4.1	18
68	A Faster Fixed-Parameter Approach to Drawing Binary Tanglegrams. Lecture Notes in Computer Science, 2009, , 38-49.	1.3	17
69	Finding Maximum Colorful Subtrees in Practice. Journal of Computational Biology, 2013, 20, 311-321.	1.6	16
70	Decomposing Metabolomic Isotope Patterns. Lecture Notes in Computer Science, 2006, , 12-23.	1.3	16
71	Patching upX-trees. Annals of Combinatorics, 1999, 3, 1-12.	0.6	15
72	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

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73	Fast alignment of fragmentation trees. Bioinformatics, 2012, 28, i265-i273.	4.1	14
74	The Generalized Robinson-Foulds Metric. Lecture Notes in Computer Science, 2013, , 156-169.	1.3	14
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	Automated bond order assignment as an optimization problem. Bioinformatics, 2011, 27, 619-625.	4.1	13
77	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
78	Efficient mass decomposition. , 2005, , .		11
79	Statistics for approximate gene clusters. BMC Bioinformatics, 2013, 14, S14.	2.6	11
80	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
81	De Novo Molecular Formula Annotation and Structure Elucidation Using SIRIUS 4. Methods in Molecular Biology, 2020, 2104, 185-207.	0.9	11
82	Swiftly Computing Center Strings. Lecture Notes in Computer Science, 2010, , 325-336.	1.3	11
83	Bad Clade Deletion Supertrees: A Fast and Accurate Supertree Algorithm. Molecular Biology and Evolution, 2017, 34, 2408-2421.	8.9	10
84	Combinatorial Approaches for Mass Spectra Recalibration. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2008, 5, 91-100.	3.0	9
85	Annotating Fragmentation Patterns. Lecture Notes in Computer Science, 2009, , 13-24.	1.3	9
86	Patchworks. Advances in Mathematics, 2001, 157, 1-21.	1.1	8
87	Extension and Robustness of Transitivity Clustering for Proteinâ€“Protein Interaction Network Analysis. Internet Mathematics, 2011, 7, 255-273.	0.7	8
88	Exact Algorithms for Cluster Editing: Evaluation and Experiments. , 2008, , 289-302.		8
89	Computation of Median Gene Clusters. Lecture Notes in Computer Science, 2008, , 331-345.	1.3	8
90	Going Weighted: Parameterized Algorithms for Cluster Editing. Lecture Notes in Computer Science, 2008, , 1-12.	1.3	8

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91	SAMPI: Protein Identification with Mass Spectra Alignments. BMC Bioinformatics, 2007, 8, 102.	2.6	7
92	Polynomial Supertree Methods Revisited. Advances in Bioinformatics, 2011, 2011, 1-21.	5.7	7
93	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
94	Interpretation of the DOME Recommendations for Machine Learning in Proteomics and Metabolomics. Journal of Proteome Research, 2022, 21, 1204-1207.	3.7	7
95	Fragmentation Trees Reloaded. Lecture Notes in Computer Science, 2015, , 65-79.	1.3	6
96	Faster Mass Decomposition. Lecture Notes in Computer Science, 2013, , 45-58.	1.3	6
97	A Note on Maximal Hierarchies. Advances in Mathematics, 2000, 151, 270-282.	1.1	5
98	Mass spectra alignments and their significance. Journal of Discrete Algorithms, 2007, 5, 714-728.	0.7	5
99	On optimal comparability editing with applications to molecular diagnostics. BMC Bioinformatics, 2009, 10, S61.	2.6	5
100	Combinatorics of aliphatic amino acids. Die Naturwissenschaften, 2011, 98, 79-86.	1.6	5
101	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
102	New Statistical Models for Copolymerization. Polymers, 2016, 8, 240.	4.5	5
103	Abundance correction for mass discrimination effects in polymer mass spectra. Rapid Communications in Mass Spectrometry, 2016, 30, 1233-1241.	1.5	5
104	Speedy Colorful Subtrees. Lecture Notes in Computer Science, 2015, , 310-322.	1.3	5
105	Collecting reliable clades using the Greedy Strict Consensus Merger. PeerJ, 2016, 4, e2172.	2.0	5
106	Mass Difference Matching Unfolds Hidden Molecular Structures of Dissolved Organic Matter. Environmental Science & Technology, 2022, 56, 11027-11040.	10.0	5
107	Swiftly Computing Center Strings. BMC Bioinformatics, 2011, 12, 106.	2.6	4
108	FlipCut Supertrees: Towards Matrix Representation Accuracy in Polynomial Time. Algorithmica, 2013, 67, 142-160.	1.3	4

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109	Identifying gene clusters by discovering common intervals in indeterminate strings. BMC Genomics, 2014, 15, S2.	2.8	4
110	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
111	A Golden Ratio Parameterized Algorithm for Cluster Editing. Lecture Notes in Computer Science, 2011, , 85-95.	1.3	4
112	Exponentially many supertrees. Applied Mathematics Letters, 2002, 15, 861-865.	2.7	3
113	Mass Spectra Alignments and Their Significance. Lecture Notes in Computer Science, 2005, , 429-441.	1.3	3
114	Computing bond orders in molecule graphs. Theoretical Computer Science, 2011, 412, 1184-1195.	0.9	3
115	Improved Fixed-Parameter Algorithms for Minimum-Flip Consensus Trees. ACM Transactions on Algorithms, 2012, 8, 1-17.	1.0	3
116	Finding Maximum Colorful Subtrees in Practice. Lecture Notes in Computer Science, 2012, , 213-223.	1.3	3
117	A note on the parameterized complexity of unordered maximum tree orientation. Discrete Applied Mathematics, 2012, 160, 1634-1638.	0.9	2
118	Computing Bond Types in Molecule Graphs. Lecture Notes in Computer Science, 2009, , 297-306.	1.3	2
119	Polynomial Supertree Methods Revisited. Lecture Notes in Computer Science, 2010, , 183-194.	1.3	2
120	Computing Fragmentation Trees from Metabolite Multiple Mass Spectrometry Data. Lecture Notes in Computer Science, 2011, , 377-391.	1.3	2
121	A FIXED-PARAMETER APPROACH FOR WEIGHTED CLUSTER EDITING. , 2007, , .		2
122	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
123	Markov Additive Chains and Applications to Fragment Statistics for Peptide Mass Fingerprinting. Lecture Notes in Computer Science, 2006, , 29-41.	1.3	2
124	Sequencing from Compomers: The Puzzle. Theory of Computing Systems, 2006, 39, 455-471.	1.1	1
125	Counting glycans revisited. Journal of Mathematical Biology, 2014, 69, 799-816.	1.9	1
126	LifeStyle-Specific-Islands (LiSSI): Integrated Bioinformatics Platform for Genomic Island Analysis. Journal of Integrative Bioinformatics, 2017, 14, .	1.5	1

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127	Exploring the Limits of the Geometric Copolymerization Model. Polymers, 2017, 9, 101.	4.5	1
128	Unrooted Supertrees. Computational Biology, 2004, , 331-351.	0.2	1
129	Determination of Glycan Structure from Tandem Mass Spectra. Lecture Notes in Computer Science, 2009, , 258-267.	1.3	1
130	FlipCut Supertrees: Towards Matrix Representation Accuracy in Polynomial Time. Lecture Notes in Computer Science, 2011, , 37-48.	1.3	1
131	Ten Times Eighteen. Journal of Information Processing, 2015, 23, 258-264.	0.4	0
132	Inferring Peptide Composition from Molecular Formulas. Lecture Notes in Computer Science, 2009, , 277-286.	1.3	0