

# Sebastian BÄjcker

## List of Publications by Year in descending order

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132  
papers

7,251  
citations

76196

40  
h-index

69108

77  
g-index

152  
all docs

152  
docs citations

152  
times ranked

6445  
citing authors

#	ARTICLE	IF	CITATIONS
1	SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. <i>Nature Methods</i> , 2019, 16, 299-302.	9.0	822
2	Searching molecular structure databases with tandem mass spectra using CSI:FingerID. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 12580-12585.	3.3	695
3	Feature-based molecular networking in the GNPS analysis environment. <i>Nature Methods</i> , 2020, 17, 905-908.	9.0	650
4	Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. <i>Nature Biotechnology</i> , 2021, 39, 462-471.	9.4	317
5	SIRIUS: decomposing isotope patterns for metabolite identification. <i>Bioinformatics</i> , 2009, 25, 218-224.	1.8	276
6	Computational mass spectrometry for metabolomics: Identification of metabolites and small molecules. <i>Analytical and Bioanalytical Chemistry</i> , 2010, 398, 2779-2788.	1.9	159
7	Fragmentation trees reloaded. <i>Journal of Cheminformatics</i> , 2016, 8, 5.	2.8	138
8	Computing Fragmentation Trees from Tandem Mass Spectrometry Data. <i>Analytical Chemistry</i> , 2011, 83, 1243-1251.	3.2	134
9	Significance estimation for large scale metabolomics annotations by spectral matching. <i>Nature Communications</i> , 2017, 8, 1494.	5.8	128
10	Base-specific fragmentation of amplified 16S rRNA genes analyzed by mass spectrometry: A tool for rapid bacterial identification. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 7039-7044.	3.3	122
11	Computational mass spectrometry for small molecules. <i>Journal of Cheminformatics</i> , 2013, 5, 12.	2.8	122
12	Critical Assessment of Small Molecule Identification 2016: automated methods. <i>Journal of Cheminformatics</i> , 2017, 9, 22.	2.8	122
13	Ion identity molecular networking for mass spectrometry-based metabolomics in the GNPS environment. <i>Nature Communications</i> , 2021, 12, 3832.	5.8	119
14	High-Throughput MALDI-TOF Discovery of Genomic Sequence Polymorphisms. <i>Genome Research</i> , 2003, 14, 126-133.	2.4	114
15	Towards <i>de novo</i> identification of metabolites by analyzing tandem mass spectra. <i>Bioinformatics</i> , 2008, 24, i49-i55.	1.8	110
16	Identifying the Unknowns by Aligning Fragmentation Trees. <i>Analytical Chemistry</i> , 2012, 84, 3417-3426.	3.2	104
17	Database-independent molecular formula annotation using Gibbs sampling through ZODIAC. <i>Nature Machine Intelligence</i> , 2020, 2, 629-641.	8.3	103
18	High-confidence structural annotation of metabolites absent from spectral libraries. <i>Nature Biotechnology</i> , 2022, 40, 411-421.	9.4	100

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19	Unbiased Transcriptional Comparisons of Generalist and Specialist Herbivores Feeding on Progressively Defenseless <i>Nicotiana attenuata</i> Plants. <i>PLoS ONE</i> , 2010, 5, e8735.	1.1	95
20	Novel Mass Spectrometry-Based Tool for Genotypic Identification of Mycobacteria. <i>Journal of Clinical Microbiology</i> , 2004, 42, 339-346.	1.8	89
21	Metabolite identification through multiple kernel learning on fragmentation trees. <i>Bioinformatics</i> , 2014, 30, i157-i164.	1.8	87
22	Computational mass spectrometry for small-molecule fragmentation. <i>TrAC - Trends in Analytical Chemistry</i> , 2014, 53, 41-48.	5.8	86
23	Partitioning biological data with transitivity clustering. <i>Nature Methods</i> , 2010, 7, 419-420.	9.0	84
24	Gene Expansion Shapes Genome Architecture in the Human Pathogen <i>Lichtheimia corymbifera</i> : An Evolutionary Genomics Analysis in the Ancient Terrestrial Mucorales (Mucoromycotina). <i>PLoS Genetics</i> , 2014, 10, e1004496.	1.5	80
25	Multiplexed discovery of sequence polymorphisms using base-specific cleavage and MALDI-TOF MS. <i>Nucleic Acids Research</i> , 2005, 33, e38-e38.	6.5	78
26	Simple but Fundamental Limitations on Supertree and Consensus Tree Methods. <i>Systematic Biology</i> , 2000, 49, 363-368.	2.7	77
27	RNase T1 mediated base-specific cleavage and MALDI-TOF MS for high-throughput comparative sequence analysis. <i>Nucleic Acids Research</i> , 2003, 31, 47e-47.	6.5	76
28	Mining molecular structure databases: Identification of small molecules based on fragmentation mass spectrometry data. <i>Mass Spectrometry Reviews</i> , 2017, 36, 624-633.	2.8	75
29	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. <i>Nature Chemical Biology</i> , 2021, 17, 146-151.	3.9	73
30	Exact Algorithms for Cluster Editing: Evaluation and Experiments. <i>Algorithmica</i> , 2011, 60, 316-334.	1.0	71
31	Current status of retention time prediction in metabolite identification. <i>Journal of Separation Science</i> , 2020, 43, 1746-1754.	1.3	71
32	New kids on the block: novel informatics methods for natural product discovery. <i>Natural Product Reports</i> , 2014, 31, 807.	5.2	64
33	A Fast and Simple Algorithm for the Money Changing Problem. <i>Algorithmica</i> , 2007, 48, 413-432.	1.0	57
34	Fast metabolite identification with Input Output Kernel Regression. <i>Bioinformatics</i> , 2016, 32, i28-i36.	1.8	57
35	<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
36	Searching molecular structure databases using tandem MS data: are we there yet?. <i>Current Opinion in Chemical Biology</i> , 2017, 36, 1-6.	2.8	53

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37	Liquid-chromatography retention order prediction for metabolite identification. <i>Bioinformatics</i> , 2018, 34, i875-i883.	1.8	52
38	Recovering Symbolically Dated, Rooted Trees from Symbolic Ultrametrics. <i>Advances in Mathematics</i> , 1998, 138, 105-125.	0.5	51
39	MSNovelist: de novo structure generation from mass spectra. <i>Nature Methods</i> , 2022, 19, 865-870.	9.0	49
40	Comprehensive cluster analysis with Transitivity Clustering. <i>Nature Protocols</i> , 2011, 6, 285-295.	5.5	47
41	Expanding the Use of Spectral Libraries in Proteomics. <i>Journal of Proteome Research</i> , 2018, 17, 4051-4060.	1.8	47
42	Current state-of-the-art of separation methods used in LC-MS based metabolomics and lipidomics. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2022, 1188, 123069.	1.2	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. <i>Bioinformatics</i> , 2003, 19, i44-i53.	1.8	42
45	EPoS: a modular software framework for phylogenetic analysis. <i>Bioinformatics</i> , 2008, 24, 2399-2400.	1.8	41
46	Exact ILP solutions for phylogenetic minimum flip problems. , 2010, , .		39
47	A golden ratio parameterized algorithm for Cluster Editing. <i>Journal of Discrete Algorithms</i> , 2012, 16, 79-89.	0.7	36
48	Bayesian networks for mass spectrometric metabolite identification via molecular fingerprints. <i>Bioinformatics</i> , 2018, 34, i333-i340.	1.8	36
49	Molecular Formula Identification with SIRIUS. <i>Metabolites</i> , 2013, 3, 506-516.	1.3	34
50	Algorithmic Aspects of Tree Amalgamation. <i>Journal of Algorithms</i> , 2000, 37, 522-537.	0.9	33
51	Computation of Median Gene Clusters. <i>Journal of Computational Biology</i> , 2009, 16, 1085-1099.	0.8	32
52	Even faster parameterized cluster deletion and cluster editing. <i>Information Processing Letters</i> , 2011, 111, 717-721.	0.4	31
53	Peak intensity prediction in MALDI-TOF mass spectrometry: A machine learning study to support quantitative proteomics. <i>BMC Bioinformatics</i> , 2008, 9, 443.	1.2	30
54	Mass spectrometry imaging of surface lipids on intact <i>Drosophila melanogaster</i> flies. <i>Journal of Mass Spectrometry</i> , 2014, 49, 223-232.	0.7	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.	1.7	28
56	De novo analysis of electron impact mass spectra using fragmentation trees. Analytica Chimica Acta, 2012, 739, 67-76.	2.6	26
57	Predicting the Presence of Uncommon Elements in Unknown Biomolecules from Isotope Patterns. Analytical Chemistry, 2016, 88, 7556-7566.	3.2	26
58	Simulating multiplexed SNP discovery rates using base-specific cleavage and mass spectrometry. Bioinformatics, 2007, 23, e5-e11.	1.8	25
59	Computing Fragmentation Trees from Metabolite Multiple Mass Spectrometry Data. Journal of Computational Biology, 2011, 18, 1383-1397.	0.8	25
60	Finding approximate gene clusters with Gecko 3. Nucleic Acids Research, 2016, 44, gkw843.	6.5	23
61	Sequencing from Compomers: Using Mass Spectrometry for DNAdenoSequencing of 200+ nt. Journal of Computational Biology, 2004, 11, 1110-1134.	0.8	22
62	Secondary ion mass spectrometry imaging and multivariate data analysis reveal coaggregation patterns of <i>Populus trichocarpa</i> leaf surface compounds on a micrometer scale. Plant Journal, 2018, 93, 193-206.	2.8	22
63	Cluster Editing. Lecture Notes in Computer Science, 2013, , 33-44.	1.0	22
64	Molecular Formula Identification Using Isotope Pattern Analysis and Calculation of Fragmentation Trees. Mass Spectrometry, 2014, 3, S0037-S0037.	0.2	20
65	Determination of Glycan Structure from Tandem Mass Spectra. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2011, 8, 976-986.	1.9	19
66	COCONUT—An Efficient Tool for Estimating Copolymer Compositions from Mass Spectra. Analytical Chemistry, 2015, 87, 5223-5231.	3.2	19
67	Decomp from interpreting Mass Spectrometry peaks to solving the Money Changing Problem. Bioinformatics, 2008, 24, 591-593.	1.8	18
68	A Faster Fixed-Parameter Approach to Drawing Binary Tanglegrams. Lecture Notes in Computer Science, 2009, , 38-49.	1.0	17
69	Finding Maximum Colorful Subtrees in Practice. Journal of Computational Biology, 2013, 20, 311-321.	0.8	16
70	Decomposing Metabolomic Isotope Patterns. Lecture Notes in Computer Science, 2006, , 12-23.	1.0	16
71	Patching up X-trees. Annals of Combinatorics, 1999, 3, 1-12.	0.3	15
72	Determination of <sup>15</sup> N-Incorporation into Plant Proteins and their Absolute Quantitation: A New Tool to Study Nitrogen Flux Dynamics and Protein Pool Sizes Elicited by Plant-Herbivore Interactions. Journal of Proteome Research, 2012, 11, 4947-4960.	1.8	15

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73	Fast alignment of fragmentation trees. <i>Bioinformatics</i> , 2012, 28, i265-i273.	1.8	14
74	The Generalized Robinson-Foulds Metric. <i>Lecture Notes in Computer Science</i> , 2013, , 156-169.	1.0	14
75	Analysis of different synthetic homopolymers by the use of a new calculation software for tandem mass spectra. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 1765-1778.	0.7	13
76	Automated bond order assignment as an optimization problem. <i>Bioinformatics</i> , 2011, 27, 619-625.	1.8	13
77	Exact and heuristic algorithms for weighted cluster editing. <i>Computational Systems Bioinformatics / Life Sciences Society Computational Systems Bioinformatics Conference</i> , 2007, 6, 391-401.	0.4	13
78	Efficient mass decomposition. , 2005, , .		11
79	Statistics for approximate gene clusters. <i>BMC Bioinformatics</i> , 2013, 14, S14.	1.2	11
80	Correcting mass shifts: A lock mass-free recalibration procedure for mass spectrometry imaging data. <i>Analytical and Bioanalytical Chemistry</i> , 2015, 407, 7603-7613.	1.9	11
81	De Novo Molecular Formula Annotation and Structure Elucidation Using SIRIUS 4. <i>Methods in Molecular Biology</i> , 2020, 2104, 185-207.	0.4	11
82	Swiftly Computing Center Strings. <i>Lecture Notes in Computer Science</i> , 2010, , 325-336.	1.0	11
83	Bad Clade Deletion Supertrees: A Fast and Accurate Supertree Algorithm. <i>Molecular Biology and Evolution</i> , 2017, 34, 2408-2421.	3.5	10
84	Combinatorial Approaches for Mass Spectra Recalibration. <i>IEEE/ACM Transactions on Computational Biology and Bioinformatics</i> , 2008, 5, 91-100.	1.9	9
85	Annotating Fragmentation Patterns. <i>Lecture Notes in Computer Science</i> , 2009, , 13-24.	1.0	9
86	Patchworks. <i>Advances in Mathematics</i> , 2001, 157, 1-21.	0.5	8
87	Extension and Robustness of Transitivity Clustering for Protein-Protein Interaction Network Analysis. <i>Internet Mathematics</i> , 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. <i>Lecture Notes in Computer Science</i> , 2008, , 331-345.	1.0	8
90	Going Weighted: Parameterized Algorithms for Cluster Editing. <i>Lecture Notes in Computer Science</i> , 2008, , 1-12.	1.0	8

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91	SAMPI: Protein Identification with Mass Spectra Alignments. BMC Bioinformatics, 2007, 8, 102.	1.2	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.	2.0	7
94	Interpretation of the DOME Recommendations for Machine Learning in Proteomics and Metabolomics. Journal of Proteome Research, 2022, 21, 1204-1207.	1.8	7
95	Fragmentation Trees Reloaded. Lecture Notes in Computer Science, 2015, , 65-79.	1.0	6
96	Faster Mass Decomposition. Lecture Notes in Computer Science, 2013, , 45-58.	1.0	6
97	A Note on Maximal Hierarchies. Advances in Mathematics, 2000, 151, 270-282.	0.5	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.	1.2	5
100	Combinatorics of aliphatic amino acids. Die Naturwissenschaften, 2011, 98, 79-86.	0.6	5
101	Comment on: "An Efficient Method to Calculate the Aggregated Isotopic Distribution and Exact Center-Masses" by Jürgen Claesen, Piotr Dittwald, Tomasz Burzykowski, Dirk Valkenburg, J. Am. Soc. Mass Spectrom. 2012, 23, 753-763. Journal of the American Society for Mass Spectrometry, 2012, 23, 1826-1827.	1.2	5
102	New Statistical Models for Copolymerization. Polymers, 2016, 8, 240.	2.0	5
103	Abundance correction for mass discrimination effects in polymer mass spectra. Rapid Communications in Mass Spectrometry, 2016, 30, 1233-1241.	0.7	5
104	Speedy Colorful Subtrees. Lecture Notes in Computer Science, 2015, , 310-322.	1.0	5
105	Collecting reliable clades using the Greedy Strict Consensus Merger. PeerJ, 2016, 4, e2172.	0.9	5
106	Mass Difference Matching Unfolds Hidden Molecular Structures of Dissolved Organic Matter. Environmental Science & Technology, 2022, 56, 11027-11040.	4.6	5
107	Swiftly Computing Center Strings. BMC Bioinformatics, 2011, 12, 106.	1.2	4
108	FlipCut Supertrees: Towards Matrix Representation Accuracy in Polynomial Time. Algorithmica, 2013, 67, 142-160.	1.0	4

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109	Identifying gene clusters by discovering common intervals in indeterminate strings. BMC Genomics, 2014, 15, S2.	1.2	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.	1.2	4
111	A Golden Ratio Parameterized Algorithm for Cluster Editing. Lecture Notes in Computer Science, 2011, , 85-95.	1.0	4
112	Exponentially many supertrees. Applied Mathematics Letters, 2002, 15, 861-865.	1.5	3
113	Mass Spectra Alignments and Their Significance. Lecture Notes in Computer Science, 2005, , 429-441.	1.0	3
114	Computing bond orders in molecule graphs. Theoretical Computer Science, 2011, 412, 1184-1195.	0.5	3
115	Improved Fixed-Parameter Algorithms for Minimum-Flip Consensus Trees. ACM Transactions on Algorithms, 2012, 8, 1-17.	0.9	3
116	Finding Maximum Colorful Subtrees in Practice. Lecture Notes in Computer Science, 2012, , 213-223.	1.0	3
117	A note on the parameterized complexity of unordered maximum tree orientation. Discrete Applied Mathematics, 2012, 160, 1634-1638.	0.5	2
118	Computing Bond Types in Molecule Graphs. Lecture Notes in Computer Science, 2009, , 297-306.	1.0	2
119	Polynomial Supertree Methods Revisited. Lecture Notes in Computer Science, 2010, , 183-194.	1.0	2
120	Computing Fragmentation Trees from Metabolite Multiple Mass Spectrometry Data. Lecture Notes in Computer Science, 2011, , 377-391.	1.0	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, .	0.3	2
123	Markov Additive Chains and Applications to Fragment Statistics for Peptide Mass Fingerprinting. Lecture Notes in Computer Science, 2006, , 29-41.	1.0	2
124	Sequencing from Compomers: The Puzzle. Theory of Computing Systems, 2006, 39, 455-471.	0.7	1
125	Counting glycans revisited. Journal of Mathematical Biology, 2014, 69, 799-816.	0.8	1
126	LifeStyle-Specific-Islands (LiSSI): Integrated Bioinformatics Platform for Genomic Island Analysis. Journal of Integrative Bioinformatics, 2017, 14, .	1.0	1



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127	Exploring the Limits of the Geometric Copolymerization Model. <i>Polymers</i> , 2017, 9, 101.	2.0	1
128	Unrooted Supertrees. <i>Computational Biology</i> , 2004, , 331-351.	0.1	1
129	Determination of Glycan Structure from Tandem Mass Spectra. <i>Lecture Notes in Computer Science</i> , 2009, , 258-267.	1.0	1
130	FlipCut Supertrees: Towards Matrix Representation Accuracy in Polynomial Time. <i>Lecture Notes in Computer Science</i> , 2011, , 37-48.	1.0	1
131	Ten Times Eighteen. <i>Journal of Information Processing</i> , 2015, 23, 258-264.	0.3	0
132	Inferring Peptide Composition from Molecular Formulas. <i>Lecture Notes in Computer Science</i> , 2009, , 277-286.	1.0	0