Theodore Alexandrov

List of Publications by Year
in descending order

99	9,751	70961 41	43802 91
papers	citations	h-index	g-index

117	117	117	11980
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking. Nature Biotechnology, 2016, 34, 828-837.	9.4	2,802
2	Mass spectral molecular networking of living microbial colonies. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, E1743-52.	3.3	804
3	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	9.0	650
4	FDR-controlled metabolite annotation for high-resolution imaging mass spectrometry. Nature Methods, 2017, 14, 57-60.	9.0	314
5	Interspecies Interactions Stimulate Diversification of the Streptomyces coelicolor Secreted Metabolome. MBio, 2013, 4, .	1.8	307
6	Critical Role of Type III Interferon in Controlling SARS-CoV-2 Infection in Human Intestinal Epithelial Cells. Cell Reports, 2020, 32, 107863.	2.9	295
7	Molecular cartography of the human skin surface in 3D. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2120-9.	3.3	288
8	Bioactivity-Based Molecular Networking for the Discovery of Drug Leads in Natural Product Bioassay-Guided Fractionation. Journal of Natural Products, 2018, 81, 758-767.	1.5	237
9	Spatial Segmentation of Imaging Mass Spectrometry Data with Edge-Preserving Image Denoising and Clustering. Journal of Proteome Research, 2010, 9, 6535-6546.	1.8	174
10	MALDI imaging mass spectrometry: statistical data analysis and current computational challenges. BMC Bioinformatics, 2012, 13, S11.	1.2	173
11	SpaceM reveals metabolic states of single cells. Nature Methods, 2021, 18, 799-805.	9.0	170
12	SARS-CoV-2 infects the human kidney and drives fibrosis in kidney organoids. Cell Stem Cell, 2022, 29, 217-231.e8.	5.2	146
13	Phenalenone-type phytoalexins mediate resistance of banana plants (Musa spp.) to the burrowing nematode Radopholus similis. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 105-110.	3.3	130
14	Spatial Metabolomics and Imaging Mass Spectrometry in the Age of Artificial Intelligence. Annual Review of Biomedical Data Science, 2020, 3, 61-87.	2.8	128
15	Exploring Three-Dimensional Matrix-Assisted Laser Desorption/Ionization Imaging Mass Spectrometry Data: Three-Dimensional Spatial Segmentation of Mouse Kidney. Analytical Chemistry, 2012, 84, 6079-6087.	3.2	122
16	Efficient spatial segmentation of large imaging mass spectrometry datasets with spatially aware clustering. Bioinformatics, 2011, 27, i230-i238.	1.8	119
17	Three-Dimensional Microbiome and Metabolome Cartography of a Diseased Human Lung. Cell Host and Microbe, 2017, 22, 705-716.e4.	5.1	111
18	The evolving field of imaging mass spectrometry and its impact on future biological research. Journal of Mass Spectrometry, 2011, 46, 209-222.	0.7	109

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19	Metabolic Profiling Directly from the Petri Dish Using Nanospray Desorption Electrospray Ionization Imaging Mass Spectrometry. Analytical Chemistry, 2013, 85, 10385-10391.	3.2	101
20	Rationale and design of the Kidney Precision Medicine Project. Kidney International, 2021, 99, 498-510.	2.6	94
21	A Review of Some Modern Approaches to the Problem of Trend Extraction. Econometric Reviews, 2012, 31, 593-624.	0.5	93
22	N-acyl Taurines and Acylcarnitines Cause an Imbalance in Insulin Synthesis and Secretion Provoking Î² Cell Dysfunction in Type 2 Diabetes. Cell Metabolism, 2017, 25, 1334-1347.e4.	7.2	87
23	3D molecular cartography using LCâ€“MS facilitated by Optimus and 'ili software. Nature Protocols, 2018, 13, 134-154.	5.5	85
24	Singleâ€cell analyses reveal SARSâ€CoVâ€2 interference with intrinsic immune response in the human gut. Molecular Systems Biology, 2021, 17, e10232.	3.2	78
25	Single-cell proteo-genomic reference maps of the hematopoietic system enable the purification and massive profiling of precisely defined cell states. Nature Immunology, 2021, 22, 1577-1589.	7.0	76
26	Microbial metabolic exchange in 3D. ISME Journal, 2013, 7, 770-780.	4.4	73
27	Biomarker discovery in MALDI-TOF serum protein profiles using discrete wavelet transformation. Bioinformatics, 2009, 25, 643-649.	1.8	68
28	Imaging mass spectrometry reveals modified forms of histone H4 as new biomarkers of microvascular invasion in hepatocellular carcinomas. Hepatology, 2013, 58, 983-994.	3.6	67
29	A reference tissue atlas for the human kidney. Science Advances, 2022, 8, .	4.7	67
30	Coupling Targeted and Untargeted Mass Spectrometry for Metabolome-Microbiome-Wide Association Studies of Human Fecal Samples. Analytical Chemistry, 2017, 89, 7549-7559.	3.2	62
31	Molecular Analysis of Model Gut Microbiotas by Imaging Mass Spectrometry and Nanodesorption Electrospray Ionization Reveals Dietary Metabolite Transformations. Analytical Chemistry, 2012, 84, 9259-9267.	3.2	59
32	A multimodal and integrated approach to interrogate human kidney biopsies with rigor and reproducibility: guidelines from the Kidney Precision Medicine Project. Physiological Genomics, 2021, 53, 1-11.	1.0	59
33	MRI-compatible pipeline for three-dimensional MALDI imaging mass spectrometry using PAXgene fixation. Journal of Proteomics, 2013, 90, 52-60.	1.2	58
34	Meta-mass shift chemical profiling of metabolomes from coral reefs. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11685-11690.	3.3	57
35	Lifestyle chemistries from phones for individual profiling. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E7645-E7654.	3.3	55
36	MALDI-imaging segmentation is a powerful tool for spatial functional proteomic analysis of human larynx carcinoma. Journal of Cancer Research and Clinical Oncology, 2013, 139, 85-95.	1.2	54

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37	Benchmark datasets for 3D MALDI- and DESI-imaging mass spectrometry. GigaScience, 2015, 4, 20.	3.3	53
38	Molecular and chemical dialogues in bacteria-protozoa interactions. Scientific Reports, 2015, 5, 12837.	1.6	51
39	Analysis and Interpretation of Imaging Mass Spectrometry Data by Clustering Mass-to-Charge Images According to Their Spatial Similarity. Analytical Chemistry, 2013, 85, 11189-11195.	3.2	48
40	MALDI imaging mass spectrometry: Discrimination of pathophysiological regions in traumatized skeletal muscle by characteristic peptide signatures. Proteomics, 2014, 14, 2249-2260.	1.3	46
41	Where imaging mass spectrometry stands: here are the numbers. Metabolomics, 2016, 12, 1.	1.4	46
42	Modelling kidney disease using ontology: insights from the Kidney Precision Medicine Project. Nature Reviews Nephrology, 2020, 16, 686-696.	4.1	45
43	Serial 3D Imaging Mass Spectrometry at Its Tipping Point. Analytical Chemistry, 2015, 87, 4055-4062.	3.2	44
44	Mass Spectrometry-Based Visualization of Molecules Associated with Human Habitats. Analytical Chemistry, 2016, 88, 10775-10784.	3.2	44
45	Testing for presence of known and unknown molecules in imaging mass spectrometry. Bioinformatics, 2013, 29, 2335-2342.	1.8	39
46	On the Importance of Mathematical Methods for Analysis of MALDI-Imaging Mass Spectrometry Data. Journal of Integrative Bioinformatics, 2012, 9, 1-11.	1.0	37
47	Spatial Molecular Architecture of the Microbial Community of a Peltigera Lichen. MSystems, 2016, 1, .	1.7	36
48	Creating a 3D microbial and chemical snapshot of a human habitat. Scientific Reports, 2018, 8, 3669.	1.6	34
49	DESI-MSI and METASPACE indicates lipid abnormalities and altered mitochondrial membrane components in diabetic renal proximal tubules. Metabolomics, 2020, 16, 11.	1.4	34
50	Digitizing mass spectrometry data to explore the chemical diversity and distribution of marine cyanobacteria and algae. ELife, 2017, 6, .	2.8	33
51	New Analysis Workflow for MALDI Imaging Mass Spectrometry: Application to the Discovery and Identification of Potential Markers of Childhood Absence Epilepsy. Journal of Proteome Research, 2012, 11, 5453-5463.	1.8	32
52	ColocML: machine learning quantifies co-localization between mass spectrometry images. Bioinformatics, 2020, 36, 3215-3224.	1.8	29
53	Progression from cirrhosis to cancer is associated with early ubiquitin postâ€translational modifications: identification of new biomarkers of cirrhosis at risk of malignancy. Journal of Pathology, 2014, 234, 452-463.	2.1	28
54	OffsampleAI: artificial intelligence approach to recognize off-sample mass spectrometry images. BMC Bioinformatics, 2020, 21, 129.	1.2	27

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55	Spatial Segmentation of MALDI FT-ICR MSI Data: A Powerful Tool to Explore the Head and Neck Tumor In Situ Lipidome. Journal of the American Society for Mass Spectrometry, 2015, 26, 36-43.	1.2	25
56	Integration of 3D multimodal imaging data of a head and neck cancer and advanced feature recognition. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 946-956.	1.1	25
57	AMASS: Algorithm for MSI Analysis by Semi-supervised Segmentation. Journal of Proteome Research, 2011, 10, 4734-4743.	1.8	24
58	Singleâ€cell transcriptomics reveals immune response of intestinal cell types to viral infection. Molecular Systems Biology, 2021, 17, e9833.	3.2	24
59	Proteomic pattern analysis discriminates among multiple sclerosisâ€“related disorders. Annals of Neurology, 2012, 71, 614-623.	2.8	23
60	Molecular and Microbial Microenvironments in Chronically Diseased Lungs Associated with Cystic Fibrosis. MSystems, 2019, 4, .	1.7	23
61	Data-Independent Microbial Metabolomics with Ambient Ionization Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2013, 24, 1167-1176.	1.2	22
62	Response Surface Methodology As a New Approach for Finding Optimal MALDI Matrix Spraying Parameters for Mass Spectrometry Imaging. Journal of the American Society for Mass Spectrometry, 2020, 31, 508-516.	1.2	22
63	Tumoral heterogeneity of hepatic cholangiocarcinomas revealed by <scp>MALDI</scp> imaging mass spectrometry. Proteomics, 2014, 14, 965-972.	1.3	21
64	Cadherin-11, Sparc-related modular calcium binding protein-2, and Pigment epithelium-derived factor are promising non-invasive biomarkers of kidney fibrosis. Kidney International, 2021, 100, 672-683.	2.6	21
65	An approach to optimize sample preparation for MALDI imaging MS of FFPE sections using fractional factorial design of experiments. Analytical and Bioanalytical Chemistry, 2016, 408, 6729-6740.	1.9	20
66	Storage Conditions of Human Kidney Tissue Sections Affect Spatial Lipidomics Analysis Reproducibility. Journal of the American Society for Mass Spectrometry, 2020, 31, 2538-2546.	1.2	20
67	DeepCycle reconstructs a cyclic cell cycle trajectory from unsegmented cell images using convolutional neural networks. Molecular Systems Biology, 2020, 16, e9474.	3.2	19
68	Public LC-Orbitrap Tandem Mass Spectral Library for Metabolite Identification. Journal of Proteome Research, 2021, 20, 2089-2097.	1.8	18
69	Using collective expert judgements to evaluate quality measures of mass spectrometry images. Bioinformatics, 2015, 31, i375-i384.	1.8	16
70	HERMES: a molecular-formula-oriented method to target the metabolome. Nature Methods, 2021, 18, 1370-1376.	9.0	16
71	Curatr: a web application for creating, curating and sharing a mass spectral library. Bioinformatics, 2018, 34, 1436-1438.	1.8	14
72	Compressed sensing in imaging mass spectrometry. Inverse Problems, 2013, 29, 125015.	1.0	13

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73	Adaptive Pixel Mass Recalibration for Mass Spectrometry Imaging Based on Locally Endogenous Biological Signals. Analytical Chemistry, 2021, 93, 4066-4074.	3.2	13
74	Application of matrixâ€assisted laser desorption/ionization mass spectrometric imaging to monitor surface changes of UVâ€irradiated poly(styrene) films. Rapid Communications in Mass Spectrometry, 2011, 25, 2809-2814.	0.7	12
75	Application of Matrix-Assisted Laser Desorption/Ionization Mass Spectrometric Imaging for Photolithographic Structuring. Analytical Chemistry, 2012, 84, 6921-6925.	3.2	12
76	PySpacell: A Python Package for Spatial Analysis of Cell Images. Cytometry Part A: the Journal of the International Society for Analytical Cytology, 2020, 97, 288-295.	1.1	12
77	Segmentation of Confocal Raman Microspectroscopic Imaging Data Using Edge-Preserving Denoising and Clustering. Analytical Chemistry, 2013, 85, 5676-5683.	3.2	9
78	Facilitating Imaging Mass Spectrometry of Microbial Specialized Metabolites with METASPACE. Metabolites, 2021, 11, 477.	1.3	9
79	Investigating the spatial distribution of growth anomalies affecting Montipora capitata corals in a 3-dimensional framework. Journal of Invertebrate Pathology, 2016, 140, 51-57.	1.5	8
80	Data-Driven Rescoring of Metabolite Annotations Significantly Improves Sensitivity. Analytical Chemistry, 2018, 90, 11636-11642.	3.2	8
81	Rapid Automated Annotation and Analysis of N-Glycan Mass Spectrometry Imaging Data Sets Using NGlycDB in METASPACE. Analytical Chemistry, 2021, 93, 13421-13425.	3.2	8
82	Histomolecular interpretation of pleomorphic adenomas of the salivary gland by matrixâ€assisted laser desorption ionization imaging and spatial segmentation. Head and Neck, 2015, 37, 1014-1021.	0.9	6
83	Metabolic decisions in development and diseaseâ€”a Keystone Symposia report. Annals of the New York Academy of Sciences, 2021, 1506, 55-73.	1.8	6
84	Rapid and Automatic Annotation of Multiple On-Tissue Chemical Modifications in Mass Spectrometry Imaging with Metaspace. Analytical Chemistry, 2022, 94, 8983-8991.	3.2	6
85	Two-Exponential Models of Gene Expression Patterns for Noisy Experimental Data. Journal of Computational Biology, 2018, 25, 1220-1230.	0.8	5
86	Probing metabolism in time and space. Science, 2020, 368, 241-242.	6.0	5
87	Patient perspectives and involvement in precision medicine research. Kidney International, 2021, 99, 511-514.	2.6	5
88	Data for spatial analysis of growth anomaly lesions on Montipora capitata coral colonies using 3D reconstruction techniques. Data in Brief, 2016, 9, 460-462.	0.5	4
89	Magnification of Label Maps With a Topology-Preserving Level-Set Method. IEEE Transactions on Image Processing, 2012, 21, 4040-4053.	6.0	3
90	Mapping the epithelialâ€“immune cell interactome upon infection in the gut and the upper airways. Npj Systems Biology and Applications, 2022, 8, 15.	1.4	3

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91	Controlled Humidity Levels for Fine Spatial Detail Information in Enzyme-Assisted N-Glycan MALDI MSI. Journal of the American Society for Mass Spectrometry, 2022, 33, 1577-1580.	1.2	3
92	The Young PI Buzz: Learning from the Organizers of the Junior Principal Investigator Meeting at ISMB-ECCB 2013. PLoS Computational Biology, 2013, 9, e1003350.	1.5	2
93	The Community Ecology of Microbial Molecules. Journal of Chemical Ecology, 2014, 40, 1161-1162.	0.9	2
94	Quantification of Duloxetine in the Bacterial Culture and Medium to Study Drug-gut Microbiome Interactions. Bio-protocol, 2021, 11, e4214.	0.2	2
95	Dependence of accuracy of ESPRIT estimates on signal eigenvalues: the case of a noisy sum of two real exponentials. Proceedings in Applied Mathematics and Mechanics, 2008, 8, 10761-10762.	0.2	1
96	Learning How to Run a Lab: Interviews with Principal Investigators. PLoS Computational Biology, 2013, 9, e1003349.	1.5	1
97	Efficient Spatial Segmentation of Hyper-spectral 3D Volume Data. Studies in Classification, Data Analysis, and Knowledge Organization, 2013, , 95-103.	0.1	0
98	Quantification reveals early dynamics in Drosophila maternal gradients. PLoS ONE, 2021, 16, e0244701.	1.1	0
99	Three Dimensional Cartography of Microbiome and Metabolome Data onto Radiological Images of the Human Lung. SSRN Electronic Journal, 0, , .	0.4	0