

# Theodore Alexandrov

## List of Publications by Year in descending order

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99  
papers

9,751  
citations

71061

41  
h-index

42364

92  
g-index

117  
all docs

117  
docs citations

117  
times ranked

11980  
citing authors

#	ARTICLE	IF	CITATIONS
1	Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking. <i>Nature Biotechnology</i> , 2016, 34, 828-837.	9.4	2,802
2	Mass spectral molecular networking of living microbial colonies. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, E1743-52.	3.3	804
3	Feature-based molecular networking in the GNPS analysis environment. <i>Nature Methods</i> , 2020, 17, 905-908.	9.0	650
4	FDR-controlled metabolite annotation for high-resolution imaging mass spectrometry. <i>Nature Methods</i> , 2017, 14, 57-60.	9.0	314
5	Interspecies Interactions Stimulate Diversification of the <i>Streptomyces coelicolor</i> Secreted Metabolome. <i>MBio</i> , 2013, 4, .	1.8	307
6	Critical Role of Type III Interferon in Controlling SARS-CoV-2 Infection in Human Intestinal Epithelial Cells. <i>Cell Reports</i> , 2020, 32, 107863.	2.9	295
7	Molecular cartography of the human skin surface in 3D. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E2120-9.	3.3	288
8	Bioactivity-Based Molecular Networking for the Discovery of Drug Leads in Natural Product Bioassay-Guided Fractionation. <i>Journal of Natural Products</i> , 2018, 81, 758-767.	1.5	237
9	Spatial Segmentation of Imaging Mass Spectrometry Data with Edge-Preserving Image Denoising and Clustering. <i>Journal of Proteome Research</i> , 2010, 9, 6535-6546.	1.8	174
10	MALDI imaging mass spectrometry: statistical data analysis and current computational challenges. <i>BMC Bioinformatics</i> , 2012, 13, S11.	1.2	173
11	SpaceM reveals metabolic states of single cells. <i>Nature Methods</i> , 2021, 18, 799-805.	9.0	170
12	SARS-CoV-2 infects the human kidney and drives fibrosis in kidney organoids. <i>Cell Stem Cell</i> , 2022, 29, 217-231.e8.	5.2	146
13	Phenalenone-type phytoalexins mediate resistance of banana plants ( <i>Musa</i> spp.) to the burrowing nematode <i>Radopholus similis</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 105-110.	3.3	130
14	Spatial Metabolomics and Imaging Mass Spectrometry in the Age of Artificial Intelligence. <i>Annual Review of Biomedical Data Science</i> , 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. <i>Analytical Chemistry</i> , 2012, 84, 6079-6087.	3.2	122
16	Efficient spatial segmentation of large imaging mass spectrometry datasets with spatially aware clustering. <i>Bioinformatics</i> , 2011, 27, i230-i238.	1.8	119
17	Three-Dimensional Microbiome and Metabolome Cartography of a Diseased Human Lung. <i>Cell Host and Microbe</i> , 2017, 22, 705-716.e4.	5.1	111
18	The evolving field of imaging mass spectrometry and its impact on future biological research. <i>Journal of Mass Spectrometry</i> , 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. <i>Analytical Chemistry</i> , 2013, 85, 10385-10391.	3.2	101
20	Rationale and design of the Kidney Precision Medicine Project. <i>Kidney International</i> , 2021, 99, 498-510.	2.6	94
21	A Review of Some Modern Approaches to the Problem of Trend Extraction. <i>Econometric Reviews</i> , 2012, 31, 593-624.	0.5	93
22	N-acyl Taurines and Acylcarnitines Cause an Imbalance in Insulin Synthesis and Secretion Provoking $\beta^2$ Cell Dysfunction in Type 2 Diabetes. <i>Cell Metabolism</i> , 2017, 25, 1334-1347.e4.	7.2	87
23	3D molecular cartography using LC-MS facilitated by Optimus and 'ili software. <i>Nature Protocols</i> , 2018, 13, 134-154.	5.5	85
24	Single-cell analyses reveal SARS-CoV-2 interference with intrinsic immune response in the human gut. <i>Molecular Systems Biology</i> , 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. <i>Nature Immunology</i> , 2021, 22, 1577-1589.	7.0	76
26	Microbial metabolic exchange in 3D. <i>ISME Journal</i> , 2013, 7, 770-780.	4.4	73
27	Biomarker discovery in MALDI-TOF serum protein profiles using discrete wavelet transformation. <i>Bioinformatics</i> , 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. <i>Hepatology</i> , 2013, 58, 983-994.	3.6	67
29	A reference tissue atlas for the human kidney. <i>Science Advances</i> , 2022, 8, .	4.7	67
30	Coupling Targeted and Untargeted Mass Spectrometry for Metabolome-Microbiome-Wide Association Studies of Human Fecal Samples. <i>Analytical Chemistry</i> , 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. <i>Analytical Chemistry</i> , 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. <i>Physiological Genomics</i> , 2021, 53, 1-11.	1.0	59
33	MRI-compatible pipeline for three-dimensional MALDI imaging mass spectrometry using PAXgene fixation. <i>Journal of Proteomics</i> , 2013, 90, 52-60.	1.2	58
34	Meta-mass shift chemical profiling of metabolomes from coral reefs. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 11685-11690.	3.3	57
35	Lifestyle chemistries from phones for individual profiling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E7645-E7654.	3.3	55
36	MALDI-imaging segmentation is a powerful tool for spatial functional proteomic analysis of human larynx carcinoma. <i>Journal of Cancer Research and Clinical Oncology</i> , 2013, 139, 85-95.	1.2	54

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37	Benchmark datasets for 3D MALDI- and DESI-imaging mass spectrometry. <i>GigaScience</i> , 2015, 4, 20.	3.3	53
38	Molecular and chemical dialogues in bacteria-protozoa interactions. <i>Scientific Reports</i> , 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. <i>Analytical Chemistry</i> , 2013, 85, 11189-11195.	3.2	48
40	MALDI imaging mass spectrometry: Discrimination of pathophysiological regions in traumatized skeletal muscle by characteristic peptide signatures. <i>Proteomics</i> , 2014, 14, 2249-2260.	1.3	46
41	Where imaging mass spectrometry stands: here are the numbers. <i>Metabolomics</i> , 2016, 12, 1.	1.4	46
42	Modelling kidney disease using ontology: insights from the Kidney Precision Medicine Project. <i>Nature Reviews Nephrology</i> , 2020, 16, 686-696.	4.1	45
43	Serial 3D Imaging Mass Spectrometry at Its Tipping Point. <i>Analytical Chemistry</i> , 2015, 87, 4055-4062.	3.2	44
44	Mass Spectrometry-Based Visualization of Molecules Associated with Human Habitats. <i>Analytical Chemistry</i> , 2016, 88, 10775-10784.	3.2	44
45	Testing for presence of known and unknown molecules in imaging mass spectrometry. <i>Bioinformatics</i> , 2013, 29, 2335-2342.	1.8	39
46	On the Importance of Mathematical Methods for Analysis of MALDI-Imaging Mass Spectrometry Data. <i>Journal of Integrative Bioinformatics</i> , 2012, 9, 1-11.	1.0	37
47	Spatial Molecular Architecture of the Microbial Community of a <i>Peltigera</i> Lichen. <i>MSystems</i> , 2016, 1, .	1.7	36
48	Creating a 3D microbial and chemical snapshot of a human habitat. <i>Scientific Reports</i> , 2018, 8, 3669.	1.6	34
49	DESI-MSI and METASPACE indicates lipid abnormalities and altered mitochondrial membrane components in diabetic renal proximal tubules. <i>Metabolomics</i> , 2020, 16, 11.	1.4	34
50	Digitizing mass spectrometry data to explore the chemical diversity and distribution of marine cyanobacteria and algae. <i>ELife</i> , 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. <i>Journal of Proteome Research</i> , 2012, 11, 5453-5463.	1.8	32
52	ColocML: machine learning quantifies co-localization between mass spectrometry images. <i>Bioinformatics</i> , 2020, 36, 3215-3224.	1.8	29
53	Progression from cirrhosis to cancer is associated with early ubiquitin post-translational modifications: identification of new biomarkers of cirrhosis at risk of malignancy. <i>Journal of Pathology</i> , 2014, 234, 452-463.	2.1	28
54	OffsampleAI: artificial intelligence approach to recognize off-sample mass spectrometry images. <i>BMC Bioinformatics</i> , 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. <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 36-43.	1.2	25
56	Integration of 3D multimodal imaging data of a head and neck cancer and advanced feature recognition. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2017, 1865, 946-956.	1.1	25
57	AMASS: Algorithm for MSI Analysis by Semi-supervised Segmentation. <i>Journal of Proteome Research</i> , 2011, 10, 4734-4743.	1.8	24
58	Single-cell transcriptomics reveals immune response of intestinal cell types to viral infection. <i>Molecular Systems Biology</i> , 2021, 17, e9833.	3.2	24
59	Proteomic pattern analysis discriminates among multiple sclerosis-related disorders. <i>Annals of Neurology</i> , 2012, 71, 614-623.	2.8	23
60	Molecular and Microbial Microenvironments in Chronically Diseased Lungs Associated with Cystic Fibrosis. <i>MSystems</i> , 2019, 4, .	1.7	23
61	Data-Independent Microbial Metabolomics with Ambient Ionization Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 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. <i>Journal of the American Society for Mass Spectrometry</i> , 2020, 31, 508-516.	1.2	22
63	Tumoral heterogeneity of hepatic cholangiocarcinomas revealed by MALDI imaging mass spectrometry. <i>Proteomics</i> , 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. <i>Kidney International</i> , 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. <i>Analytical and Bioanalytical Chemistry</i> , 2016, 408, 6729-6740.	1.9	20
66	Storage Conditions of Human Kidney Tissue Sections Affect Spatial Lipidomics Analysis Reproducibility. <i>Journal of the American Society for Mass Spectrometry</i> , 2020, 31, 2538-2546.	1.2	20
67	DeepCycle reconstructs a cyclic cell cycle trajectory from unsegmented cell images using convolutional neural networks. <i>Molecular Systems Biology</i> , 2020, 16, e9474.	3.2	19
68	Public LC-Orbitrap Tandem Mass Spectral Library for Metabolite Identification. <i>Journal of Proteome Research</i> , 2021, 20, 2089-2097.	1.8	18
69	Using collective expert judgements to evaluate quality measures of mass spectrometry images. <i>Bioinformatics</i> , 2015, 31, i375-i384.	1.8	16
70	HERMES: a molecular-formula-oriented method to target the metabolome. <i>Nature Methods</i> , 2021, 18, 1370-1376.	9.0	16
71	Curatr: a web application for creating, curating and sharing a mass spectral library. <i>Bioinformatics</i> , 2018, 34, 1436-1438.	1.8	14
72	Compressed sensing in imaging mass spectrometry. <i>Inverse Problems</i> , 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. <i>Analytical Chemistry</i> , 2021, 93, 4066-4074.	3.2	13
74	Application of matrix-assisted laser desorption/ionization mass spectrometric imaging to monitor surface changes of UV-irradiated poly(styrene) films. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 2809-2814.	0.7	12
75	Application of Matrix-Assisted Laser Desorption/Ionization Mass Spectrometric Imaging for Photolithographic Structuring. <i>Analytical Chemistry</i> , 2012, 84, 6921-6925.	3.2	12
76	PySpacell: A Python Package for Spatial Analysis of Cell Images. <i>Cytometry Part A: the Journal of the International Society for Analytical Cytology</i> , 2020, 97, 288-295.	1.1	12
77	Segmentation of Confocal Raman Microspectroscopic Imaging Data Using Edge-Preserving Denoising and Clustering. <i>Analytical Chemistry</i> , 2013, 85, 5676-5683.	3.2	9
78	Facilitating Imaging Mass Spectrometry of Microbial Specialized Metabolites with METASPACE. <i>Metabolites</i> , 2021, 11, 477.	1.3	9
79	Investigating the spatial distribution of growth anomalies affecting <i>Montipora capitata</i> corals in a 3-dimensional framework. <i>Journal of Invertebrate Pathology</i> , 2016, 140, 51-57.	1.5	8
80	Data-Driven Rescoring of Metabolite Annotations Significantly Improves Sensitivity. <i>Analytical Chemistry</i> , 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. <i>Analytical Chemistry</i> , 2021, 93, 13421-13425.	3.2	8
82	Histomolecular interpretation of pleomorphic adenomas of the salivary gland by matrix-assisted laser desorption ionization imaging and spatial segmentation. <i>Head and Neck</i> , 2015, 37, 1014-1021.	0.9	6
83	Metabolic decisions in development and disease—a Keystone Symposia report. <i>Annals of the New York Academy of Sciences</i> , 2021, 1506, 55-73.	1.8	6
84	Rapid and Automatic Annotation of Multiple On-Tissue Chemical Modifications in Mass Spectrometry Imaging with Metaspac. <i>Analytical Chemistry</i> , 2022, 94, 8983-8991.	3.2	6
85	Two-Exponential Models of Gene Expression Patterns for Noisy Experimental Data. <i>Journal of Computational Biology</i> , 2018, 25, 1220-1230.	0.8	5
86	Probing metabolism in time and space. <i>Science</i> , 2020, 368, 241-242.	6.0	5
87	Patient perspectives and involvement in precision medicine research. <i>Kidney International</i> , 2021, 99, 511-514.	2.6	5
88	Data for spatial analysis of growth anomaly lesions on <i>Montipora capitata</i> coral colonies using 3D reconstruction techniques. <i>Data in Brief</i> , 2016, 9, 460-462.	0.5	4
89	Magnification of Label Maps With a Topology-Preserving Level-Set Method. <i>IEEE Transactions on Image Processing</i> , 2012, 21, 4040-4053.	6.0	3
90	Mapping the epithelial-immune cell interactome upon infection in the gut and the upper airways. <i>Npj Systems Biology and Applications</i> , 2022, 8, 15.	1.4	3

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91	Controlled Humidity Levels for Fine Spatial Detail Information in Enzyme-Assisted <i>N</i> -Glycan MALDI MSI. <i>Journal of the American Society for Mass Spectrometry</i> , 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. <i>PLoS Computational Biology</i> , 2013, 9, e1003350.	1.5	2
93	The Community Ecology of Microbial Molecules. <i>Journal of Chemical Ecology</i> , 2014, 40, 1161-1162.	0.9	2
94	Quantification of Duloxetine in the Bacterial Culture and Medium to Study Drug-gut Microbiome Interactions. <i>Bio-protocol</i> , 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. <i>Proceedings in Applied Mathematics and Mechanics</i> , 2008, 8, 10761-10762.	0.2	1
96	Learning How to Run a Lab: Interviews with Principal Investigators. <i>PLoS Computational Biology</i> , 2013, 9, e1003349.	1.5	1
97	Efficient Spatial Segmentation of Hyper-spectral 3D Volume Data. <i>Studies in Classification, Data Analysis, and Knowledge Organization</i> , 2013, , 95-103.	0.1	0
98	Quantification reveals early dynamics in <i>Drosophila</i> maternal gradients. <i>PLoS ONE</i> , 2021, 16, e0244701.	1.1	0
99	Three Dimensional Cartography of Microbiome and Metabolome Data onto Radiological Images of the Human Lung. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0