

# Theodore Alexandrov

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

103  
papers

5,892  
citations

34  
h-index

76  
g-index

117  
ext. papers

7,974  
ext. citations

8.1  
avg, IF

5.74  
L-index

#	Paper	IF	Citations
103	Mapping the epithelial-immune cell interactome upon infection in the gut and the upper airways.. <i>Npj Systems Biology and Applications</i> , <b>2022</b> , 8, 15	5	0
102	SARS-CoV-2 infects the human kidney and drives fibrosis in kidney organoids.. <i>Cell Stem Cell</i> , <b>2021</b> ,	18	24
101	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> , <b>2021</b> , 22, 1577-1589	19.1	14
100	HERMES: a molecular-formula-oriented method to target the metabolome. <i>Nature Methods</i> , <b>2021</b> , 18, 1370-1376	21.6	3
99	Quantification of Duloxetine in the Bacterial Culture and Medium to Study Drug-gut Microbiome Interactions. <i>Bio-protocol</i> , <b>2021</b> , 11, e4214	0.9	
98	Single-cell analyses reveal SARS-CoV-2 interference with intrinsic immune response in the human gut. <i>Molecular Systems Biology</i> , <b>2021</b> , 17, e10232	12.2	23
97	Facilitating Imaging Mass Spectrometry of Microbial Specialized Metabolites with METASPACE. <i>Metabolites</i> , <b>2021</b> , 11,	5.6	1
96	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> , <b>2021</b> , 53, 1-11	3.6	21
95	Public LC-Orbitrap Tandem Mass Spectral Library for Metabolite Identification. <i>Journal of Proteome Research</i> , <b>2021</b> , 20, 2089-2097	5.6	6
94	Adaptive Pixel Mass Recalibration for Mass Spectrometry Imaging Based on Locally Endogenous Biological Signals. <i>Analytical Chemistry</i> , <b>2021</b> , 93, 4066-4074	7.8	5
93	SpaceM reveals metabolic states of single cells. <i>Nature Methods</i> , <b>2021</b> , 18, 799-805	21.6	33
92	Single-cell transcriptomics reveals immune response of intestinal cell types to viral infection. <i>Molecular Systems Biology</i> , <b>2021</b> , 17, e9833	12.2	4
91	Metabolic decisions in development and disease-a Keystone Symposia report. <i>Annals of the New York Academy of Sciences</i> , <b>2021</b> ,	6.5	1
90	Quantification reveals early dynamics in Drosophila maternal gradients. <i>PLoS ONE</i> , <b>2021</b> , 16, e0244701	3.7	
89	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> , <b>2021</b> , 100, 672-683	9.9	1
88	Rapid Automated Annotation and Analysis of N-Glycan Mass Spectrometry Imaging Data Sets Using NGlycDB in METASPACE. <i>Analytical Chemistry</i> , <b>2021</b> , 93, 13421-13425	7.8	1
87	Critical Role of Type III Interferon in Controlling SARS-CoV-2 Infection in Human Intestinal Epithelial Cells. <i>Cell Reports</i> , <b>2020</b> , 32, 107863	10.6	186

86	OffsampleAI: artificial intelligence approach to recognize off-sample mass spectrometry images. <i>BMC Bioinformatics</i> , <b>2020</b> , 21, 129	3.6	15
85	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> , <b>2020</b> , 31, 508-516	3.5	10
84	DESI-MSI and METASPACE indicates lipid abnormalities and altered mitochondrial membrane components in diabetic renal proximal tubules. <i>Metabolomics</i> , <b>2020</b> , 16, 11	4.7	12
83	Spatial Metabolomics and Imaging Mass Spectrometry in the Age of Artificial Intelligence. <i>Annual Review of Biomedical Data Science</i> , <b>2020</b> , 3, 61-87	5.6	49
82	DeepCycle reconstructs a cyclic cell cycle trajectory from unsegmented cell images using convolutional neural networks. <i>Molecular Systems Biology</i> , <b>2020</b> , 16, e9474	12.2	6
81	ColocML: machine learning quantifies co-localization between mass spectrometry images. <i>Bioinformatics</i> , <b>2020</b> , 36, 3215-3224	7.2	12
80	PySpacell: A Python Package for Spatial Analysis of Cell Images. <i>Cytometry Part A: the Journal of the International Society for Analytical Cytology</i> , <b>2020</b> , 97, 288-295	4.6	5
79	Modelling kidney disease using ontology: insights from the Kidney Precision Medicine Project. <i>Nature Reviews Nephrology</i> , <b>2020</b> , 16, 686-696	14.9	17
78	Feature-based molecular networking in the GNPS analysis environment. <i>Nature Methods</i> , <b>2020</b> , 17, 905-906	20.8	207
77	Storage Conditions of Human Kidney Tissue Sections Affect Spatial Lipidomics Analysis Reproducibility. <i>Journal of the American Society for Mass Spectrometry</i> , <b>2020</b> , 31, 2538-2546	3.5	9
76	Probing metabolism in time and space. <i>Science</i> , <b>2020</b> , 368, 241-242	33.3	2
75	Molecular and Microbial Microenvironments in Chronically Diseased Lungs Associated with Cystic Fibrosis. <i>MSystems</i> , <b>2019</b> , 4,	7.6	15
74	Creating a 3D microbial and chemical snapshot of a human habitat. <i>Scientific Reports</i> , <b>2018</b> , 8, 3669	4.9	23
73	Bioactivity-Based Molecular Networking for the Discovery of Drug Leads in Natural Product Bioassay-Guided Fractionation. <i>Journal of Natural Products</i> , <b>2018</b> , 81, 758-767	4.9	134
72	3D molecular cartography using LC-MS facilitated by Optimus and Tli software. <i>Nature Protocols</i> , <b>2018</b> , 13, 134-154	18.8	53
71	Curatr: a web application for creating, curating and sharing a mass spectral library. <i>Bioinformatics</i> , <b>2018</b> , 34, 1436-1438	7.2	10
70	Two-Exponential Models of Gene Expression Patterns for Noisy Experimental Data. <i>Journal of Computational Biology</i> , <b>2018</b> , 25, 1220-1230	1.7	4
69	Data-Driven Rescoring of Metabolite Annotations Significantly Improves Sensitivity. <i>Analytical Chemistry</i> , <b>2018</b> , 90, 11636-11642	7.8	5

68	Coupling Targeted and Untargeted Mass Spectrometry for Metabolome-Microbiome-Wide Association Studies of Human Fecal Samples. <i>Analytical Chemistry</i> , <b>2017</b> , 89, 7549-7559	7.8	46
67	N-acyl Taurines and Acylcarnitines Cause an Imbalance in Insulin Synthesis and Secretion Provoking $\beta$ Cell Dysfunction in Type 2 Diabetes. <i>Cell Metabolism</i> , <b>2017</b> , 25, 1334-1347.e4	24.6	52
66	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> , <b>2017</b> , 114, 11685-11690	11.5	37
65	Three-Dimensional Microbiome and Metabolome Cartography of a Diseased Human Lung. <i>Cell Host and Microbe</i> , <b>2017</b> , 22, 705-716.e4	23.4	74
64	FDR-controlled metabolite annotation for high-resolution imaging mass spectrometry. <i>Nature Methods</i> , <b>2017</b> , 14, 57-60	21.6	167
63	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> , <b>2017</b> , 1865, 946-956	4	19
62	Digitizing mass spectrometry data to explore the chemical diversity and distribution of marine cyanobacteria and algae. <i>ELife</i> , <b>2017</b> , 6,	8.9	26
61	Investigating the spatial distribution of growth anomalies affecting <i>Montipora capitata</i> corals in a 3-dimensional framework. <i>Journal of Invertebrate Pathology</i> , <b>2016</b> , 140, 51-57	2.6	5
60	Lifestyle chemistries from phones for individual profiling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2016</b> , 113, E7645-E7654	11.5	41
59	Spatial Molecular Architecture of the Microbial Community of a Lichen. <i>MSystems</i> , <b>2016</b> , 1,	7.6	22
58	Where imaging mass spectrometry stands: here are the numbers. <i>Metabolomics</i> , <b>2016</b> , 12, 1	4.7	32
57	Mass Spectrometry-Based Visualization of Molecules Associated with Human Habitats. <i>Analytical Chemistry</i> , <b>2016</b> , 88, 10775-10784	7.8	38
56	Data for spatial analysis of growth anomaly lesions on coral colonies using 3D reconstruction techniques. <i>Data in Brief</i> , <b>2016</b> , 9, 460-462	1.2	2
55	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> , <b>2016</b> , 408, 6729-40	4.4	17
54	Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking. <i>Nature Biotechnology</i> , <b>2016</b> , 34, 828-837	44.5	1566
53	Molecular cartography of the human skin surface in 3D. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2015</b> , 112, E2120-9	11.5	237
52	Serial 3D imaging mass spectrometry at its tipping point. <i>Analytical Chemistry</i> , <b>2015</b> , 87, 4055-62	7.8	41
51	Histomolecular interpretation of pleomorphic adenomas of the salivary gland by matrix-assisted laser desorption ionization imaging and spatial segmentation. <i>Head and Neck</i> , <b>2015</b> , 37, 1014-21	4.2	5

50	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> , <b>2015</b> , 26, 36-43	3.5	24
49	Molecular and chemical dialogues in bacteria-protozoa interactions. <i>Scientific Reports</i> , <b>2015</b> , 5, 12837	4.9	34
48	Benchmark datasets for 3D MALDI- and DESI-imaging mass spectrometry. <i>GigaScience</i> , <b>2015</b> , 4, 20	7.6	45
47	Using collective expert judgements to evaluate quality measures of mass spectrometry images. <i>Bioinformatics</i> , <b>2015</b> , 31, i375-84	7.2	13
46	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> , <b>2014</b> , 111, 105-10	11.5	97
45	MALDI imaging mass spectrometry: discrimination of pathophysiological regions in traumatized skeletal muscle by characteristic peptide signatures. <i>Proteomics</i> , <b>2014</b> , 14, 2249-60	4.8	37
44	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> , <b>2014</b> , 234, 452-63	9.4	25
43	Tumoral heterogeneity of hepatic cholangiocarcinomas revealed by MALDI imaging mass spectrometry. <i>Proteomics</i> , <b>2014</b> , 14, 965-72	4.8	18
42	The community ecology of microbial molecules. <i>Journal of Chemical Ecology</i> , <b>2014</b> , 40, 1161-2	2.7	2
41	Data-independent microbial metabolomics with ambient ionization mass spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , <b>2013</b> , 24, 1167-76	3.5	19
40	MRI-compatible pipeline for three-dimensional MALDI imaging mass spectrometry using PAXgene fixation. <i>Journal of Proteomics</i> , <b>2013</b> , 90, 52-60	3.9	49
39	Metabolic profiling directly from the Petri dish using nanospray desorption electrospray ionization imaging mass spectrometry. <i>Analytical Chemistry</i> , <b>2013</b> , 85, 10385-91	7.8	80
38	Analysis and interpretation of imaging mass spectrometry data by clustering mass-to-charge images according to their spatial similarity. <i>Analytical Chemistry</i> , <b>2013</b> , 85, 11189-95	7.8	40
37	Microbial metabolic exchange in 3D. <i>ISME Journal</i> , <b>2013</b> , 7, 770-80	11.9	63
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> , <b>2013</b> , 139, 85-95	4.9	51
35	Segmentation of confocal Raman microspectroscopic imaging data using edge-preserving denoising and clustering. <i>Analytical Chemistry</i> , <b>2013</b> , 85, 5676-83	7.8	8
34	Interspecies interactions stimulate diversification of the <i>Streptomyces coelicolor</i> secreted metabolome. <i>MBio</i> , <b>2013</b> , 4,	7.8	242
33	The young PI buzz: learning from the organizers of the Junior Principal Investigator Meeting at ISMB-ECCB 2013. <i>PLoS Computational Biology</i> , <b>2013</b> , 9, e1003350	5	0

32	Compressed sensing in imaging mass spectrometry. <i>Inverse Problems</i> , <b>2013</b> , 29, 125015	2.3	9
31	Testing for presence of known and unknown molecules in imaging mass spectrometry. <i>Bioinformatics</i> , <b>2013</b> , 29, 2335-42	7.2	27
30	Efficient Spatial Segmentation of Hyper-spectral 3D Volume Data. <i>Studies in Classification, Data Analysis, and Knowledge Organization</i> , <b>2013</b> , 95-103	0.2	
29	Imaging mass spectrometry reveals modified forms of histone H4 as new biomarkers of microvascular invasion in hepatocellular carcinomas. <i>Hepatology</i> , <b>2013</b> , 58, 983-94	11.2	59
28	Magnification of label maps with a topology-preserving level-set method. <i>IEEE Transactions on Image Processing</i> , <b>2012</b> , 21, 4040-53	8.7	2
27	Application of matrix-assisted laser desorption/ionization mass spectrometric imaging for photolithographic structuring. <i>Analytical Chemistry</i> , <b>2012</b> , 84, 6921-5	7.8	12
26	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> , <b>2012</b> , 11, 5453-63	5.6	30
25	A Review of Some Modern Approaches to the Problem of Trend Extraction. <i>Econometric Reviews</i> , <b>2012</b> , 31, 593-624	1.1	67
24	Exploring three-dimensional matrix-assisted laser desorption/ionization imaging mass spectrometry data: three-dimensional spatial segmentation of mouse kidney. <i>Analytical Chemistry</i> , <b>2012</b> , 84, 6079-87	7.8	101
23	MALDI imaging mass spectrometry: statistical data analysis and current computational challenges. <i>BMC Bioinformatics</i> , <b>2012</b> , 13 Suppl 16, S11	3.6	145
22	Molecular analysis of model gut microbiotas by imaging mass spectrometry and nanodesorption electrospray ionization reveals dietary metabolite transformations. <i>Analytical Chemistry</i> , <b>2012</b> , 84, 9259-67	7.8	50
21	Proteomic pattern analysis discriminates among multiple sclerosis-related disorders. <i>Annals of Neurology</i> , <b>2012</b> , 71, 614-23	9.4	18
20	Mass spectral molecular networking of living microbial colonies. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2012</b> , 109, E1743-52	11.5	593
19	On the Importance of Mathematical Methods for Analysis of MALDI-Imaging Mass Spectrometry Data. <i>Journal of Integrative Bioinformatics</i> , <b>2012</b> , 9, 1-11	3.8	29
18	AMASS: algorithm for MSI analysis by semi-supervised segmentation. <i>Journal of Proteome Research</i> , <b>2011</b> , 10, 4734-43	5.6	22
17	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> , <b>2011</b> , 25, 2809-14	2.2	9
16	The evolving field of imaging mass spectrometry and its impact on future biological research. <i>Journal of Mass Spectrometry</i> , <b>2011</b> , 46, 209-22	2.2	99
15	Efficient spatial segmentation of large imaging mass spectrometry datasets with spatially aware clustering. <i>Bioinformatics</i> , <b>2011</b> , 27, i230-8	7.2	94

14	Spatial segmentation of imaging mass spectrometry data with edge-preserving image denoising and clustering. <i>Journal of Proteome Research</i> , <b>2010</b> , 9, 6535-46	5.6	151
13	Biomarker discovery in MALDI-TOF serum protein profiles using discrete wavelet transformation. <i>Bioinformatics</i> , <b>2009</b> , 25, 643-9	7.2	59
12	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> , <b>2009</b> , 8, 10761-10762	0.2	1
11	Critical role of type III interferon in controlling SARS-CoV-2 infection, replication and spread in primary human intestinal epithelial cells		18
10	A reference tissue atlas for the human kidney		2
9	Single-cell transcriptomics reveals immune response of intestinal cell types to viral infection		4
8	Single-cell analyses reveal SARS-CoV-2 interference with intrinsic immune response in the human gut		6
7	Spatial single-cell profiling of intracellular metabolomes in situ		19
6	Recognizing off-sample mass spectrometry images with machine and deep learning		4
5	METASPACE: A community-populated knowledge base of spatial metabolomes in health and disease		21
4	ColocAI: artificial intelligence approach to quantify co-localization between mass spectrometry images		2
3	Feature-based Molecular Networking in the GNPS Analysis Environment		29
2	A Multimodal and Integrated Approach to Interrogate Human Kidney Biopsies with Rigor and Reproducibility: The Kidney Precision Medicine Project		1
1	Single-cell proteo-genomic reference maps of the hematopoietic system enable the purification and massive profiling of precisely defined cell states		2