

## European Molecular Biology Laboratory

EMBL

### Staff

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### Summary

EMBL has contributed with the Spatial Metabolomics use-case. EMBL has collaborated with IBM Research and URV. EMBL has used Lithops to implement a new serverless version of the cloud software METASPACE for spatial metabolomics, deployed it onto IBM Cloud, and started using it in production since April 2021. EMBL has provided feedback and multiple bug reports to IBM Research and URV on Lithops and on the use of Lithops on IBM Cloud. Together with IBM Research, EMBL has conceived and implemented the hybrid version of METASPACE combining the use of Lithops for serverless computing and virtual machines. EMBL has helped IBM Research to test the novel infrastructure CodeEngine integrating serverless capabilities and virtual machines.

### Publications (Total: 3)

Katja Ovchinnikova, Vitaly Kovalev, [Lachlan Stuart](#), [Theodore Alexandrov](#)

**OffsampleAI: artificial intelligence approach to recognize off-sample mass spectrometry images**

BMC Bioinformatics (2020) 21:129

[link](#)

[Theodore Alexandrov](#)

**Spatial Metabolomics and Imaging Mass Spectrometry in the Age of Artificial Intelligence**

Annu. Rev. Biomed. Data Sci. 2020. 3:61–87

[link](#)

Rocca RL, Kune C, Tiquet M, Stuart LS, [Alexandrov T](#), De Pauw E, Quinton L

**Using Biological Signals for Mass Recalibration of Mass Spectrometry Imaging Data**

Analytical Chemistry, 93(8), 4066-4074

[link](#)

## Open source repositories (Total: 1)

Lithops METASPACE <https://github.com/metaspaces2020/Lithops-METASPACE>

## Dissemination activities (Total: 63)

Talks by Theodore Alexandrov at conferences presenting in detail the serverless version of METASPACE, its capabilities and advantages (2)

1. KubeCon, May 2021, online
2. IBM Cloud Native Day, Apr 2021, online

Talks by Theodore Alexandrov at conferences and workshops, highlighting the serverless version of METASPACE used in production (30):

1. Nature Conference Bioengineering Solutions for Biology & Medicine (BIOENG), Jul 2022, Munich, DE
2. Single-Cell Proteomics Conference (SCP2022), Jun 2022, Boston, MA, USA (virtual)
3. Int. Conference of TRR179 Viral Hepatitis and Beyond, May 2022, Freiburg, DE
4. Spatial Omics SEMM Roundtable at the European School of Molecular Medicine, May 2022, Milan, IT (virtual)
5. EMBL-EBI Training Course "Introduction to Metabolomics Analysis", May 2022, Hinxton, UK
6. Mitteldeutsche Laborkonferenz (Central Germany Diagnostics Lab Conference), May 2022, Weimar, DE
7. 2nd Annual Mini Symposium in Human Genetics, Apr 2022, Emory Uni / Atlanta, GA, USA
8. Spatial Biology UK, Apr 2022, London, UK
9. Science in Immunology Meeting at King's College London, Apr 2022, London, UK (keynote)
10. Chan-Zuckerberg Initiative (CZI) workshop on single-cell proteomics and metabolomics, Apr 2022, US / virtual
11. Spatial Biology – Accelerating Translational Research & Clinical Applications, Apr 2022, UK / virtual
12. Korean Metabolomics Society, Apr 2022, South Korea / virtual (keynote)

13. Online Round Table of Institute of Biomedicine of Seville, Mar 2022, Sevilla, ES / virtual
14. MINDS Workshop, Mar 2022, Wiesbaden, DE
15. Certificate of Advanced Studies In Personalized Molecular Oncology, Feb 2022, Basel, CH / virtual
16. German Mass Cytometry User Forum, Jan 2022, Berlin, DE / online
17. Int. Conference of SFB1335 Aberrant Immune Signals in Cancer, Dec 2021, Munich, DE / online
18. Pioneers in Omics, Dec 2021, virtual
19. BigData World Congress and Genomics Live, Nov 2021, Basel, CH
20. Int. Mass Spectrometry Imaging Conference (OurCon), Oct 2021, UK / virtual (keynote)
21. CSHL meeting on Mechanisms of Metabolic Signaling, Oct 2021, Cold Spring Harbor, NY, USA
22. Oz Single-Cell Brisbane Meeting, Oct 2021, Brisbane, AU / online
23. Plant Cell Atlas Symposium, Oct 2021, online
24. de.NBI Summer School Mass Spec Omics Data, Sep 2021, online
25. 2<sup>nd</sup> Workshop on Metabolomics in Chronic Inflammation Barrier Diseases, Sep 2021, Kiel, DE
26. ISMB, CompMS session, July 2021, online (keynote)
27. ICI-CIVIS Summer School in Immuno-Oncology, July 2021, Marseille, FR (keynote)
28. Metabolomics Conference, June 2021, online (keynote)
29. IHMC International Human Microbiome Consortium Congress, Jun 2021, ES / online (keynote)
30. LIPID MAPS Spring School, Apr 2021, online

Talks by Theodore Alexandrov at conferences and workshops, highlighting the cloud software METASPACE and the potential of using serverless computing for spatial metabolomics (**29**):

1. Keystone Symposium on Metabolic Decisions in Development & Disease, Mar 2021, US / online
2. VIZBI Visualizing Biological Data Workshop, Mar 2021, DE / online
3. 72nd AACC Annual Scientific Meeting, Dec 2020, US / online
4. START-HD Single-Cell and Spatial Omics Workshop, Nov 2020, Heidelberg / online

5. Lipid Droplets Workshop, Nov 2020, online
6. BigData World Congress and Genomics Live, Nov 2020, Basel, CH / online
7. FASTest 2020 E-lecture for Dutch Tenure Track Network & COAST, Sep 2020, online
8. Spatial Omics, Joint Zoom Seminar Series <http://spatialomics.net>, Sep 2020, online
9. 12<sup>th</sup> Annual Congress in Clinical Mass Spectrometry (MSACL), May 2020, online (keynote)
10. Webinar in Sphingolipids Biology, May 2020, online
11. Certificate of Advanced Studies In Personalized Molecular Oncology, Feb 2020, Basel, CH
12. 2<sup>nd</sup> Annual Symposium of ITMO on Immunology, Inflammation, Infectiology and Microbiology (I3M), Feb 2020, Lille, FR (keynote)
13. EMBO-EMBL Symposium Metabolism Meets Epigenetics, Nov 2019, Heidelberg, DE
14. ASMS Asilomar Conference on Mass Spectrometry, Oct 2019, Pacific Grove, CA, USA
15. Munich Metabolomics Meeting, Oct 2019, Munich, DE (keynote)
16. Bayer MS Imaging Workshop, Oct 2019, Berlin, DE
17. EMBO Workshop Lipid Function in Health and Disease, Sep 2019, Dresden, DE
18. EMBL Partnership Conference Perspectives in Translational Medicine, Sep 2019, Barcelona, ES
19. German Pharmaceutical Society Symposium, Sep 2019, Heidelberg, DE (keynote)
20. M4I Workshop on Mass Spectrometry Imaging, Sep 2019, Maastricht, NL
21. Metabolomics Conference, Jun 2019, the Hague, NL (keynote)
22. BMBF e:Med Summer School, May 2019, Castle Ringberg, DE
23. Highlight Symposium at European Molecular Imaging Meeting, March 2019, Glasgow, UK
24. VIB Conference Metabolism in Cancer and Stromal Cells, Nov 2018, Leuven, BE (plenary)
25. Clinical Proteomics Symposium, Nov 2018, Barcelona, ES
26. OurCon & IMSS conference on Imaging Mass Spectrometry, Nov 2018, Charleston, NC, USA
27. Multi-Omics Seminar Tour by ThermoFisher Scientific, Oct 2018, Wiesloch, DE
28. AI and Blockchain for Healthcare Forum at Based Life Conference, Sep 2018, Basel, CH

29. Helmholtz Conference on Engineering Biomedical & Metabolic Breakthroughs, Jul 2018, Venice, IT

#### Blog posts (1)

- Together with IBM Research on the potential of using IBM CloudFunctions infrastructure and PyWren/Lithops for spatial metabolomics:  
<https://www.ibm.com/cloud/blog/decoding-dark-molecular-matter-in-spatial-metabolomics-with-ibm-cloud-functions>

#### Websites (1):

- METASPACE: <http://metaspace2020.eu>

#### Exploitation Activities (Total: 2)

- 1) EMBL has deployed the Lithops version of METASPACE in production (<http://metaspace2020.eu>) in April 2021. Since then, it was used for processing more than 8.000 datasets, that represents more than 40% of datasets processed by METASPACE since its start in 2015.
- 2) EMBL has launched an incubation phase of the startup SpaceM for spatial single-cell metabolomics for drug discovery that was enabled by the serverless version of METASPACE. The incubation phase is funded by the BioStudio program of the BioInnovation Institute in Copenhagen, Denmark, an incubator and foundation in the space of life sciences and health technologies. The startup is hosted at the BioInnovation Institute, is scientifically coordinated by Theodore Alexandrov, and already involves 4 staff members, with hiring of two more staff members currently on the way.

#### Collaborations (Total: 2)

EMBL has collaborated mainly with:

- 1) IBM Research, on jointly developing the Lithops version of METASPACE, on deploying it onto IBM Cloud, on implementing the hybrid version of METASPACE involving Lithops and virtual machines, and on testing the novel IBM serverless infrastructure CodeEngine
- 2) URV, on providing feedback, bug reports, and performing testing of Lithops