



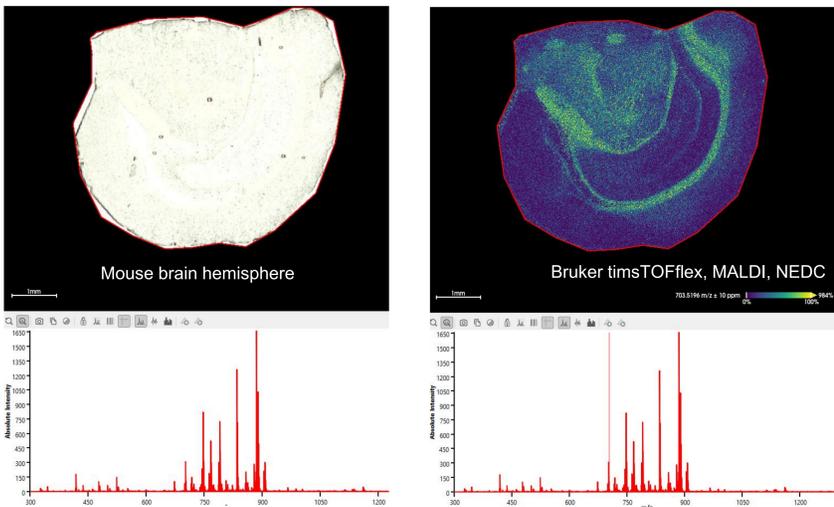
Truthful visualizations for mass spectrometry imaging enable high spatial resolution interactive m/z mapping and exploration

Jacob GILDENBLAT ¹ and Jens PAHNKE ^{1,2,3,4,5}

¹ Pahnke Lab, ² University of Oslo and University Hospital Oslo, Norway; ³ University Medical Center and University of Lübeck, INUM, Germany; ⁴ University of Latvia, Department of Neuromedicine and Neuroscience, Riga, Latvia; ⁵ University of Tel Aviv, G. S. Wise Faculty of Life Sciences, Department of Neuroscience, Biochemistry and Biophysics, Israel

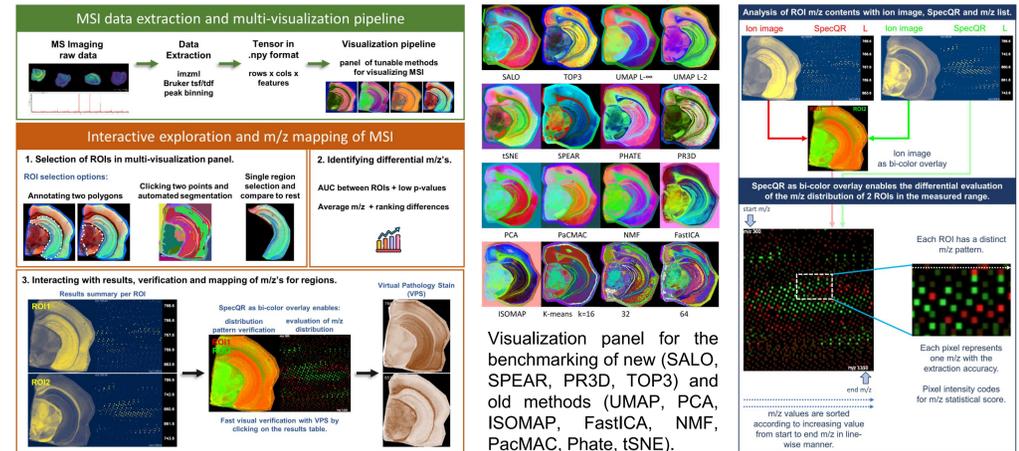
1. Motivation and Rationale

We have identified an urgent need for computationally sophisticated, interactive, and automated visualization tools specifically designed for MSI analysis that employ dimensionality reduction (DR) methods to preserve global data structure. New DR methods beyond UMAP need high global structure preservation to view small localized details, e.g., like Alzheimer plaques, cancer cells, etc.



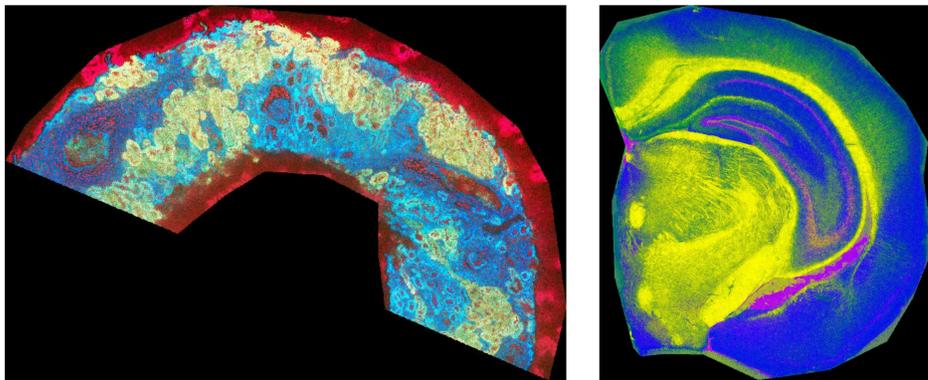
2. MSI-VISUAL workflow and SpecQR

MSI-VISUAL provides a framework to visualize high-dim MSI datasets with time consuming methods preserving the global data structure (SALO/SPEAR) but also with ultra fast methods for fast browsing and assessment (PR3D, TOP3). The SpecQR diagram enables data m/z characteristics visualization of ROIs.



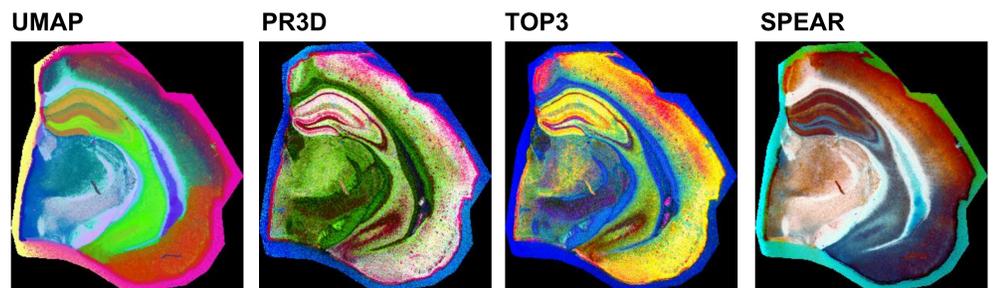
3. Saliency optimization (SALO)

Novel optimization that considers changes in both many or few m/z values and optimizes for high global structure preservation by preserving the ranks of distances from reference points.



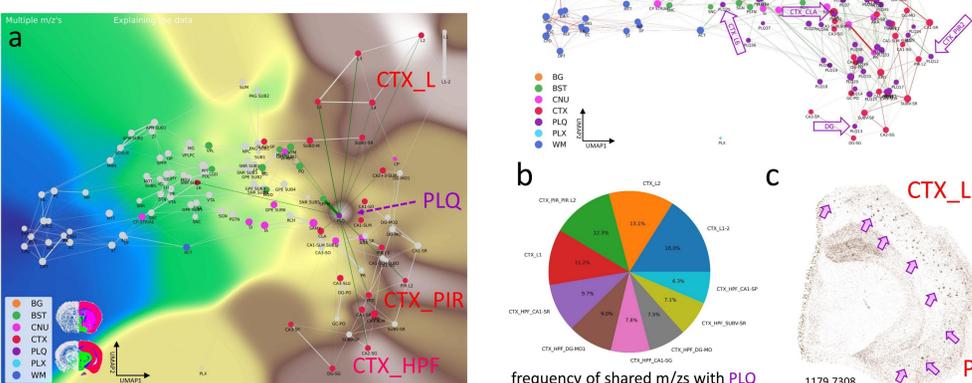
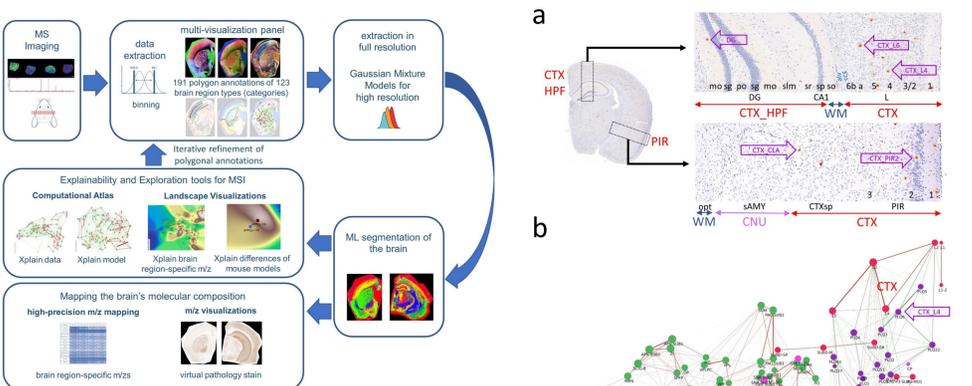
4. PR3D / TOP3

Development of ultra light-weight and fast visualization methods enabling fast MSI data assessment for, e.g. diagnostic purposes.



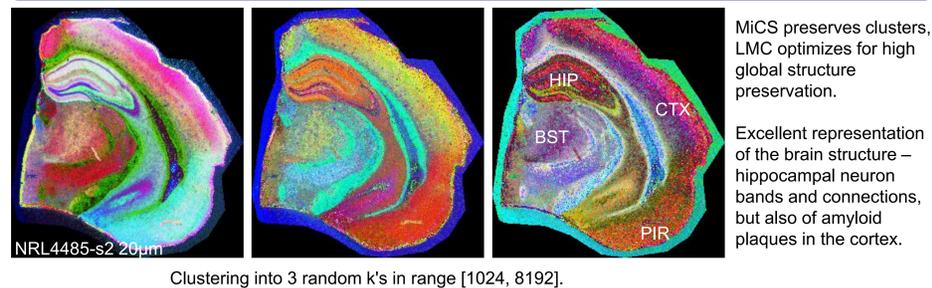
6. MSI-ATLAS

Analysis of lipidomics data from mouse brain tissue by employing the new visualizations and brain region annotations, ML-assisted segmenting of the brain, data exploration, landscape visualization, and m/z mapping.



5. MiCS/LMC DR method

We introduce two complementary objectives that jointly preserve global geometry and local structure. Landmark Mantel Correlation (LMC) aligns high- and low-dimensional distances with respect to a small set of landmarks, providing an efficient global constraint. Multi-resolution Cluster Supervision (MiCS) promotes local fidelity by encouraging cluster assignments—estimated across multiple resolutions—to remain predictable after projection.



7. Upcoming work: MiCS/LMC to train NN

Using deep neural networks for ultra scale visualization of 5µm-resolution brain images with our novel dimensionality reduction methods as an objective to train.

