BOOK OF ABSTRACTS

XI COLLOQUIUM CHEMOMETRICUM MEDITERRANEUM

27-30 JUNE 2023
PADOVA - ITALY

EXPLORING SEA BASS MULTIOMIC IMAGES FOR SPATIALLY RESOLVED TRANSCRIPTOMICS AND METABOLOMICS

Albert Menéndez-Pedriza[1], Mercedes Blázquez[2], Eduardo Chicano-Gálvez[3], Laia Navarro-Martín[1] and Joaquim Jaumot[1]

Addresses:

1. Institute of Environmental Assessment and Water Research – Spanish National Research Council (IDAEA-CSIC), Department of Environmental Chemistry, Jordi Girona 18-26, E08034. Barcelona, Spain.

2. Institute of Marine Sciences – Spanish National Research Council (ICM-CSIC), Passeig Maritim 37-49, E08003 Barcelona, Spain.

3. Maimonides Institute of Biomedical Research of Córdoba (IMIBIC), Mass Spectrometry and Molecular Imaging Unit (IMSMI), Avda Menéndez Pidal s/n, E14004 Córdoba, Spain

E-mail: joaquim.jaumot@idaea.csic.es

Omic studies traditionally focused on analyzing metabolites from homogenized samples, resulting in the loss of morphological information. However, new techniques like mass spectrometry imaging (MSI)[1], useful for proteomics and metabolomics studies, and spatial transcriptomics[2] (ST) have emerged, allowing for the acquisition of images while retaining morphological information. MSI generates an image containing a mass spectrum in each pixel whereas ST allows for the identification of gene expression information and its location at the image. These techniques provide both structural information that characterizes and identifies the compounds or genes found on the surface of the samples, and morphological information that represents where these compounds are located.

The latest developments involve the fusion of multiomic images, which can be achieved by generating transcriptomic, proteomic, and/or metabolomic images from consecutive tissue sections[3]. Targeted studies analyze pre-defined molecules, while untargeted methods consider the entire dataset, using multivariate analysis to reveal most of the biological information and generate new hypotheses.

In this study, we present chemometric strategies for analyzing spatial transcriptomics and metabolomics (lipidomics) images, with the goal of identifying spatial regions with similar behavior and determining the genes or chemical compounds

responsible for the observed differentiation. To illustrate our approach, we consider several testicular sections from European sea bass testicular sections in which different developmental stages, according to the maturation level, could be identified.

Our chemometric workflow includes several key stages, such as data import, quality control, filtering, and dimensionality reduction. We apply chemometrics tools for resolution and clustering to identify regions of interest and their potential markers. Figure 1 shows distribution maps for spatial transcriptomics and lipidomics for two sea bass testicular sections, revealing distinct clusters characterized by specific molecular signatures.

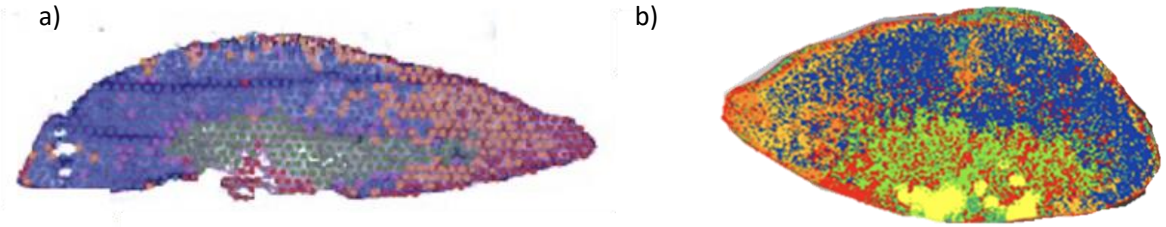

Figure 1. Clustering images obtained for a) spatial transcriptomics and b) spatial lipidomics

Finally, we aim to obtain a holistic picture by fusing the spatial multiomics images. However, the fusion process presents certain drawbacks from a chemometric perspective, such as ensuring correspondence between images (i.e., similarity between consecutive tissue slices) and addressing differences in spatial resolution used by the different spatial omics approaches. Therefore, an additional step of pixel size homogenization is required before the final chemometric analysis and the different considered approaches will be discussed.

Acknowledgements

Grant PID2021-122929OB-C33 funded by MCIN/AEI/10.13039/501100011033 and, as appropriate, by "ERDF A way of making Europe.

References

1. McDonnell, L.A., Heeren, R.M.A. Imaging mass spectrometry (**2007**) Mass Spectrometry Reviews, **26** (4), pp. 606-643.
2. Ståhl, P.L., Salmén, F., et al. Visualization and analysis of gene expression in tissue sections by spatial transcriptomics (**2016**) Science, **353** (6294), pp. 78-82.
3. Porta Siegel, T., Hamm, G., et al. Mass Spectrometry Imaging and Integration with Other Imaging Modalities for Greater Molecular Understanding of Biological Tissues (**2018**) Molecular Imaging and Biology, **20** (6), pp. 888-901.