Master thesis project opportunity:

Developing tools for spatial correlation in mass spectrometry imaging

A mass spectrometer determines the mass to charge ratio (m/z) and detects the intensity of each m/z to produce a mass spectrum (figure 1). Mass spectrometry imaging (MSI) can be used to spatially map molecules directly to the surface of a sample, such as a thin tissue section. This is performed by recorded mass spectra in pixels all across the sample surface. Following, selected m/z values can be mapped in 2D to generate an ion image. By mapping the intensity of a specific m/z (or molecules) in biological samples we can gain insights into the chemical importance in biological systems.

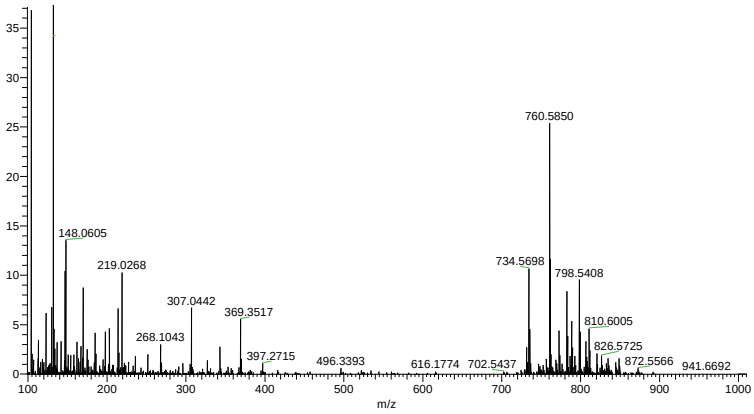

Figure 1. Example of a mass spectrum from mouse brain tissue. The mass to charge value (m/z) is on the x-axis and the relative abundance on the y-axis.

The data in MSI has many levels with every pixel containing a mass spectrum, such as the one in Figure 1, which can contain thousands of detected species. Traditionally, selected and predefined m/z values are used to generate ion images. However, as a result, most of the information is not used. Therefore, new or improved ways to spatially correlate non-targeted m/z values can contribute to more efficient investigation of the data, such as finding m/z values that co-localize in particular areas of the sample. By spatially correlating m/z values in depth, insights from the MSI data can be gained in a simpler and more robust way.

One approach to use is clustering, which there are plenty of suggested workflows for in the literature.[1–3] Alternative approaches should also be considered and the applicability should be evaluated in several ways, including i) robustness ii) specificity and iii) computational cost. Ultimately, the chosen approach should be robust to noise and artefacts, enable identification and separation of morphological regions, and be of moderate computational cost. With such an approach we foresee extraction of new chemical information from our existing data set.

The project will be supervised by Prof. Ingela Lanekoff at the Dept. of Chemistry-BMC. If you are interested in the project or have questions about it, please email Ingela.lanekoff@kemi.uu.se.

References

1. Verbeeck, N., Caprioli, R. M. & Van de Plas, R. Unsupervised machine learning for exploratory data analysis in imaging mass spectrometry. *Mass Spectrom. Rev.* **39**, 245–291 (2020).
2. Zhang, W. *et al.* Spatially aware clustering of ion images in mass spectrometry imaging data using deep learning. *Anal. Bioanal. Chem.* **413**, 2803–2819 (2021).
3. Smets, T. *et al.* Evaluation of Distance Metrics and Spatial Autocorrelation in Uniform Manifold Approximation and Projection Applied to Mass Spectrometry Imaging Data. *Anal. Chem.* **91**, 5706–5714 (2019).