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Tutorial SC4

Exploring advanced ToF-SIMS data analysis techniques

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ToF-SIMS imaging produces very complex information. Each pixel or voxel contains a complete mass spectrum, containing elemental, inorganic and organic secondary ion signals. Additionally, the energy from the primary ion beam leads to the fragmentation of molecular ions, resulting in a multitude of correlated fragment ion signals. In biological samples, where numerous molecules share similar building blocks, this complexity is further amplified. Moreover, the intensity of secondary ions is affected by the chemical environment, referred to as the matrix effect, which introduces non-linearity. As a result, only relative quantitation is achievable. The lack of robust data analysis tools capable of handling the large and complex datasets generated by ToF-SIMS and similar hyperspectral techniques has limited their use. Consequently, many researchers have been working on the development of advanced multivariate data analysis tools to aid in the interpretation of ToF-SIMS image data. This development is vital considering the continuous growth of these datasets, because improved spatial and mass resolution, larger field of view imaging, and additional MS/MS data thanks to recent technological developments.

This tutorial will first delve into the intricacies of ToF-SIMS image data and the analytical challenges it presents. We will then dive into unsupervised machine learning methods like PCA and clustering algorithms to tackle dimensionality reduction and image segmentation. Additionally, we will take a look at supervised machine learning algorithms for addressing classification tasks. Since this is a short seminar, our focus will be on equipping you with a foundational understanding of these techniques and their practical applications to ToF-SIMS data. The aim of this tutorial is to empower new ToF-SIMS users with the essential knowledge and tools to embark on exploring this aspect of our chosen research field themselves.