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POINT OF VIEW

Chemical Imaging – Is an Image Always Worth a Thousand Spectra?

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Chemical images can be described as distribution maps that correlate the chemical information of an element or molecule, such as mass-to-charge ratio (*m/z*) or wavelength, with its intensity and/or concentration in a given sample. These images are usually obtained by mass spectrometry (MS) or optical spectroscopy techniques, where hundreds or thousands of spectra are initially acquired and dedicated image processing software is employed to construct and edit the final pictures, as well as selecting and annotating regions of interest in a sample, performing calibration procedures, etc.

Mass spectrometry imaging (preferably abbreviated as MSI, to distinguish it from ion mobility spectrometry – IMS) is currently the most employed chemical imaging strategy, as can be noticed in the most recently published papers. Depending on the selected ionization technique, molecular or elemental images can be acquired. For molecular MSI, the classical matrix-assisted laser desorption/ionization (MALDI) is generally applied for imaging lipids, peptides and proteins, and the ambient ionization technique desorption electrospray ionization (DESI) is commonly applied for visualizing lipid distribution. In terms of elemental MSI, laser ablation inductively coupled plasma (LA-ICP) is undoubtedly the technique of choice, although nano-secondary ion mass spectrometry (nanoSIMS) can also be applied.

Considering optical spectroscopy, the main techniques used nowadays are Raman and near-infrared radiation – NIR – spectroscopy for molecular imaging, and Synchrotron radiation X-ray fluorescence – SRXRF – and laser-induced breakdown spectroscopy – LIBS – for elemental imaging. Amongst these techniques, the best spatial resolutions are generally achieved by SRXRF (elemental imaging) and Raman spectroscopy (molecular imaging).

Analytical chemistry advances in chemical imaging allow the acquisition of images with high spatial resolution, which is particularly interesting when studying specific regions or cell structures in a biological sample. For instance, in a Parkinson's disease model, LA-ICP-MS images with good spatial resolution make the distinction of specific mouse brain regions possible and, consequently, the association of metal ion concentrations to each region,[1] which is a relevant result considering micro-local metal speciation in neurodegenerative diseases.

Nevertheless, there are some drawbacks in chemical imaging that demand further analytical development, such as the long analysis time and the lack of certified reference materials for quantitative analysis and method validation, as well as open-source software with advanced multivariate statistical analysis tools.

Another obstacle to overcome concerns the integration of elemental and molecular imaging results. Since 2009, when one of the first review articles regarding the combination of these imaging approaches

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in a synergistic way was proposed by Becker and Jakubowski,[2] until more recently described in reviews from 2020[3] and 2021,[4] it has been possible to realize that there is still much work to be done in this field. This is mostly due to the fact that each imaging technique provides different spatial resolutions, making image superposition difficult, and also the absence of software and algorithms that allow the integration of different data sets in order to obtain trustworthy results and produce relevant study hypotheses. Besides that, the instrumentation for chemical imaging is rather costly and usually research groups are specialized in either molecular or elemental imaging.

With these considerations, it is important to emphasize that the community involved in chemical imaging research should focus not only on the quality of the generated images in terms of resolution but also, if they are indeed worth a thousand spectra, on interpretation of the initial questions in a deep and holistic manner. After all, the main objective of chemical imaging is that the images represent how the process in question (disease, treatment, contamination, genetic modification, etc.) locally affects the system (biological, environmental, pharmaceutical sample) under study and, then, provide solutions for solving problems in different areas, such as forensic, environmental and life sciences.

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Alessandra Sussulini received her Ph.D. in Analytical Chemistry from the University of Campinas (UNICAMP), Brazil. Since 2014, she has been an Assistant Professor at the same university. Previously, she was a postdoctoral fellow of the Alexander von Humboldt Foundation at the Jülich Research Centre, Germany. Her current research activities are mainly focused on the application of mass spectrometry-based multi-omics strategies (proteomics, metabolomics, lipidomics and metallomics) to study psychiatric/neurodegenerative diseases and their treatments. CV