Commentary

iMedPub Journals
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American Journal of Pharmacology and Pharmacotherapeutics
ISSN 2393-8862

2023
Vol.10 No.3:160

Spatial Metabolomics Principles and their Utilisation in Cancer Research

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Received date: August 18, 2023, Manuscript No. IPAPP-23-18023; **Editor assigned date:** August 21, 2023, PreQC No. IPAPP-23-18023 (PQ); **Reviewed date:** September 04, 2023, QC No. IPAPP-23-18023; **Revised date:** September 11, 2023, Manuscript No. IPAPP-23-18023 (R); **Published date:** September 18, 2023, DOI: 10.36648/2393-8862.10.3.160

Citation: Azmeh C (2023) Spatial Metabolomics Principles and their Utilisation in Cancer Research. Am J Pharmacol Pharmacother Vol. 10 No. 3: 160.

Description

Mass Spectrometry Imaging (MSI) is a new method in cancer metabolomics. Desorption Electrospray Ionisation (DESI) and Matrix-Assisted Laser Desorption Ionisation (MALDI) are two methods of ionisation. MSI are complementary techniques to identify hundreds of metabolites in space with close to single-cell resolution. This technology leap enables research focusing on tumor heterogeneity, cancer cell plasticity, and the communication signals between cancer and stromal cells in the Tumor Micro Environment (TME). Currently, knowledge is generated using spatial metabolomics in fundamental cancer research.

Metabolic rewiring is an important modulator of cancer progression, which may contribute to treatment resistance highlighting the need for assessing metabolites and metabolic conversion rates. Bulk metabolite analysis by mass spectrometry combined with chromatographic methods has been the state-of-the-art method to analyze metabolites in cancer research. Metabolites are extracted from bio fluids, cells, or tissues. Yielding information on the average metabolite concentration in the sample. However, deeper knowledge on the spatial distribution and architecture of metabolism within the tumor lost.

Mass Spectrometry Imaging (MSI) is a label-free technique that allows spatial mapping of hundreds of metabolites and drugs directly from a tissue section. It allows to assess tumor heterogeneity, cancer cell plasticity and cancer-stromal cell communication in the tumor microenvironment and Desorption Electrospray Ionization (DESI) in cancer research by highlighting recent advances and remaining challenges.

Visualization of Metabolites

MALDI-MSI allows spatial visualization of metabolites and in particular lipids in tissues using laser ionization. A matrix is applied directly on tissue sections, forming co-crystals with metabolites. Upon radiation with the laser beam, the matrix is ionized (addition or loss of a proton) and charges are transferred to the metabolites, resulting in desorption and ionization. The choice of the matrix determines the acquisition mode. MALDI works by combining a sample usually a large molecule like a protein or peptide with a matrix compound. This mixture is then coated onto a metal plate.

The desorbed and ionized molecules are then accelerated into a mass analyzer, where they are classified according to their mass-to-charge ratio (m/z). Notably, the material used to embed the tissues and the MALDI matrices can interfere with metabolites detection.

Sample preparation proper sample preparation is crucial for accurate metabolite detection. It involves techniques like extraction, purification, and derivatization to isolate and concentrate the metabolites of interest.

Mass Spectrometry (MS) is a key analytical technique used in metabolomics. It involves ionizing molecules and measuring their mass-to-charge ratios. Techniques like Liquid Chromatography-Mass Spectrometry (LC-MS) and Gas Chromatography-Mass Spectrometry (GC-MS) are commonly employed. Retention time alignment in LC-MS, retention time alignment is essential to ensure that corresponding peaks in different samples are aligned. This is critical for accurate quantification.

Peak detection and integration after data acquisition, software tools are used to detect peaks corresponding to different metabolites and integrate the area under each peak to quantify the metabolites.

Tumor Metabolism

MSI has been used to infer the spatial complexity of tumors. In glioblastoma-derived xenografts, an inverse abundance of ATP and acylcarnitine was detected. Resected human brain tissue slices showed differences in antioxidant metabolites, nucleotides, and fatty acid composition of tumors versus peritumor material. Additionally, it was shown that glycogen, a multibranched polysaccharide of glucose that serves as energy storage, displays high MSI has been used to infer the spatial complexity of tumors. In glioblastoma-derived xenografts, an inverse abundance of ATP and acylcarnitine was detected.

Additionally, MSI is becoming a broadly applicable spatial technology. However, some bottlenecks remain and need to be resolved the spatial resolution delivered by current instruments do not allow to infer subcellular distribution of metabolites

without destruction into elements by X-ray fluorescence and nano SIMS. Furthermore, the nature of MSI analysis requires simultaneous ablation of all ions from a pixel, which limits the identification of metabolites with similar m/z ratio.