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## **Metabolomics and Imaging**

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Metabolome reflects the sum of all life processes within the cell-tissue-organ, belonging to all or any the systems that constitute the individual and it refers to metabolites included during a cell, tissue or organism. Since metabolites are various, in terms of chemical species and concentrations, it's necessary to conduct metabolite analysis with a spread of various analytical techniques. Imaging is that the main a part of these modern diagnosis pathways. A narrative review of all the relevant papers known to the authors was conducted, researching the PubMed database. Considering this last definition of the multimodal in vivo - in vitro approach, an important and versatile diagnostic procedure is often considered the foremost recent and crucial innovation in modern diagnostics: Nuclear resonance (NMR).For the in vitro application, NMR has become a crucial tool for metabolomics. Metabolomics is defined because the quantitative and chemical analysis of an outsized number of metabolites that are intermediate or final products of all the metabolic pathways during a biological system. Metabolomics aims to get a worldwide understanding of living organisms to a deeper level than has thus far been achieved through genomics and proteomics. This property is of great clinical importance in light of recent definitions of health and disease.

Multicellular tumor spheroids (MCTS) have gained increasing attention in cancer research because they'll closely mimic some physiological characteristics of solid tumors. MCTS are considered as a useful three-dimensional cell model for evaluating the effect of exogenous molecules on tumor progression. However, little is understood about the metabolic response in MCTS after exposure to exogenous molecules. Herein, we applied metabolomics combined with

MALDI-mass spectrometry imaging (MSI) to research the proliferation of threedimensional MDA-MB-231 carcinoma cell spheroids treated with bisphenol S (BPS). MSI data revealed that BPS, a standard environmental contaminant, penetrated MCTS in 5 min and gradually localized within the core of MCTS within 4 h. Metabolomic data demonstrated that BPS exposure induced significant changes within the levels of 28 metabolites that are involved in several pathways, including purine metabolism and therefore the tricarboxylic acid cycle. The MSI results showed that three upregulated metabolites (ATP, ADP, and AMP) acting major roles in energy supply distributed within the proliferative zone of cell spheroids, further indicating the proliferative response of MDA-MB-231 cell spheroids caused by BPS exposure. One downregulated metabolite (xanthine) related to reactive oxidative stress was found to localize toward the inner region of cell spheroids. These MSI results demonstrated that the rise of energy supply within the outer layer of cell spheroids could be liable for BPS-induced proliferative response. Taken together, this integrated method might offer a more accurate and intuitive assessment for the effect of exogenous molecules on cancer progression.

## Conclusion

This review highlights the workflow of a typical metabolomics study and summarizes the foremost up-to-date results obtained from the newest in vivo imaging techniques and their technologies, focusing on the longer term perspective of in vivo MRS Metabolomics.

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