

Advancements in bioinformatics for lipidomics study: searching for systemic biomarkers in patients with breast cancer.

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## INTRODUCTION

Lipids play crucial roles as biomarkers in breast cancer due to their involvement in tumor microenvironment and cancer-associated metabolic processes. Lipidomic studies have highlighted variations in free fatty acids and phospholipids in breast tumor samples, offering potential to differentiate between subtypes of breast cancers. This approach promises a deeper insight into tumor-specific metabolic or membrane composition alterations, paving the way for precise lipid biomarker panels and enhancing precision medicine for breast cancer diagnosis.

## OBJECTIVES

The aim of this study was to identify and quantify potential lipid biomarkers in plasma samples from various breast cancer types, utilizing optimized bioanalytical, chemometric, and bioinformatics methodologies.

## MATERIALS AND METHODS

Lipid extraction process employed reagents such as methanol, chloroform, and MTBE, along with internal standards. Three extraction methods: Bligh & Dyer, Matyash Traditional, and Modified Matyash, were utilized, each with specific protocols for plasma analysis. Unarget LC-MS/MS analysis was performed using a UHPLC coupled with a Sciex Triple-TOF 5600+ mass spectrometer. Data processing utilized MS-DIAL<sup>TM</sup> and MultiQuant<sup>TM</sup> software, with standardized parameters for the lipidomic analysis.

## DISCUSSION AND RESULTS

The study yielded valuable insights into selecting an appropriate lipidomic extraction methodology and bioinformatics tools for biomarker investigation. Over 200 lipids were accurately identified and quantified, providing a robust platform for comparing lipid profiles between healthy individuals and breast cancer patients. This holds promise for uncovering significant biomarkers with diagnostic and therapeutic implications.

## CONCLUSION

Selecting a robust lipid extraction methodology spanning diverse lipid classes proved crucial for identifying potential biomarkers. This enabled the identification of potential biomarkers for future exploration, which could be translated into new diagnostic methodologies and therapeutic applications. Additionally, the significance of bioinformatic analysis via MS-DIAL and its databases cannot be overstated, as they facilitated the rapid and accurate identification of these lipids

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