Perspective
Volume 15:4, 2022

Journal of Computer Science & Systems Biology

ISSN: 0974-7230 Open Access

A Scheduled Multiple Reaction Monitoring Method for High Throughput Lipidomics

Esther Leuenberger*

Department of Information Science, University of Melbourne, Australia

Introduction

Lipids are a diverse group of biomolecules that play an important role in the body's normal functioning, including cellular homeostasis, cell signalling, and energy storage. Obesity and diabetes, cardiovascular disease, cancer, and other metabolic diseases are all associated with dysregulation of lipid homeostasis. Cell, tissue, and biofluid lipid compositions are complex, reflecting a wide range of concentrations of different lipid classes and structural diversity within lipid species. Although the precise number of distinct lipids present in cells is unknown, it is believed that the cellular lipidome consists of over 1000 different lipid species, each with multiple structural isomers [1-3].

Traditional methods for identifying lipids, such as Thin Layer Chromatography (TLC), Nuclear Magnetic Resonance (NMR), and soft ionizations techniques (field desorption, chemical ionization, or fast atom bombardment), are limited in sensitivity and accuracy, making them unsuitable for comprehensive lipidomics studies. Recent advances in lipidomics using Electrospray Ionization-Mass Spectrometry (ESI-MS) have allowed for the accurate identification of a large number of lipid species from various biological sources. For greater coverage with increasing sensitivity and specificity, lipids have been analysed in both positive and negative ion modes in a single mass spectrometric scan using untargeted or targeted approaches.

Description

The limitations of an untargeted lipidomics approach in terms of lipid species characterization, processing time, and bias toward the detection of high-abundance lipids are greatly reduced when using a targeted approach *via* Multiple Reaction Monitoring (MRM). A scheduled-MRM, in which MRM transitions are monitored only around the expected retention time of the eluting lipid species, allows for the monitoring of a greater number of MRM transitions in a single MS acquisition. A variable Retention Time (RT) window width tailored to each lipid species could shorten the analysis time of a schedule-MRM method, increasing throughput. Furthermore, the quality of the peaks can be improved by varying the dwell time weightage for each transition while keeping the cycle time constant. Regardless of the elution window, assigning a low dwell time weightage to high abundant compounds and a high dwell time weightage to less abundant compounds aids in accommodating a large number of transitions in a single run with improved data quality [4,5].

We present a rapid and sensitive targeted lipidomics method capable of identifying more than 1000 lipid species in a single MS run-time of 24 minutes by optimising a combination of scheduled-MRM, variable RT window, and dwell time weightage. This method can be used as a first screening method in large-scale lipidomics experiments. This method was also used to screen lipid species altered in vitamin B12 deficiency in the Indian population. The variable retention time window and variable dwell time weightage for all transitions were optimised using scheduled MRM Builder, an Excel-based tool from Sciex. The tool's operation is based on the chromatographic peak's variation in width, area, and retention time. Each MRM transition can have its own RT window thanks to variable retention time window width. Wider windows are assigned to analytes with greater run-to-run variation or wider peak widths.

Conclusion

We compared the area under the curve obtained in XIC (extracted ion chromatogram) for different lipid species in advanced MRM (scheduled MRM with variable-RTW and relative-DTW) with sMRM and MRM after optimising dwell weight and RT window. In all three types of scans, all of the LC and MS parameters were the same. Lipids were extracted from pooled plasma (from five samples) on three different days and subjected to MS analysis with five technical replicates on each day. The study (which was part of a larger study) was designed to identify plasma lipids that were altered due to vitamin B12 deficiency in the study population. According to their plasma vitamin B12 levels, apparently healthy people were divided into two groups. The participants gave their informed consent. The CSIR-IGIB institutional ethical committee approved the study. Individuals with vitamin B12 levels less than 150 pg/mL were considered deficient, while those with levels between 400 and 800 pg/mL were considered normal.

We used the method to try to identify the plasma lipid species that are altered due to vitamin B12 deficiency. Vitamin B12 is a micronutrient found primarily in animal products, and a lack of it has been linked to lipid imbalance. When all lipid classes were considered together, there was no significant change. When individual lipid species within the classes were compared using differential expression analysis, it was discovered that 55 lipid species were altered between the two groups.

References

1. Al-Hashimi, Nessreen A and Yasser H.A. Hussein. "Ab initio study on the formation of triiodide CT complex from the reaction of iodine with 2, 3-diaminopyridine." *Spectrochim Acta A Mol Biomol Spectrosc* 75 (2010): 198-202.
2. Hoven, Van Den and John. "Data architecture: Standards for the effective enterprise." *Manag Inf Syst* 21 (2004): 61.
3. Ylimäki, Tanja and Veikko Halttunen. "Method engineering in practice: A case of applying the Zachman framework in the context of small enterprise architecture oriented projects." *Inf Knowl Syst Manag* 5 (2005): 189-209.
4. Sowa, John F and John A. Zachman. "Extending and formalizing the framework for information systems architecture." *IBM Syst J* 31 (1992): 590-616.
5. Iyer, Bala and R. Gottlieb. "The Four-Domain Architecture: An approach to support enterprise architecture design." *IBM Syst J* 43 (2004): 587-597.

***Address for Correspondence:** Esther Leuenberger, Department of Information Science, University of Melbourne, Australia, E mail: EstherLeuenberger50@gmail.com*

Received: 07-Apr-2022, Manuscript No. jcsb-22-66583; **Editor assigned:** 09-Apr-2022, Pre QC No. P-66583; **Reviewed:** 23-Apr-2022, QC No. 66583; **Revised:** 28-Apr-2022, Manuscript No. R-66583; **Published:** 05-May-2022, DOI: 10.37421/0974-7230.2022.15.410.

How to cite this article: Leuenberger, Esther. "A Scheduled Multiple Reaction Monitoring Method for High Throughput Lipidomics." J Comput Sci Syst Biol 15 (2022): 410.