

Integrated Quantification and Multivariate Analysis Workbench System for Phospholipids

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1 Introduction

Phospholipids are essential components of cell membrane, which consists of variety of phospholipid molecular species with different chain lengths, unsaturated bound positions and polar groups. A mass spectrometer (MS) is widely used to identify and to quantify phospholipid molecular species in a mixture due to its high sensitivity. To observe expression difference among organs or in time-series data of developmental process, quantification must be performed for multiple samples, and the results tend to produce a high dimensional data. To simplify experimental data processing and analyzing step, we developed an integrated workbench system for phospholipid quantification and analysis.

2 System Overview

2.1. Key Features

(1) Data Management with Native XML Database

All information is stored in XML format for interoperability with other systems. An open source native XML database "Xindice" [1] is used to store and retrieve XML files efficiently.

(2) Personal Workspace

Users can have their own workspaces authorized by login ID and password.

(3) Web-based application

Since the user interface is a web browser, there is basically no limitation for client operating system. It also allows users to access their workspaces from anywhere via the Internet.

(4) Integrated Data Analysis by Simple Operation

The workbench system provides functionality to compare raw quantification data or to perform multivariate analysis.

2.2. System Design

The workbench system consists of three modules, and figure 1 describes the relationship between them. The system currently runs on a Linux operating system.

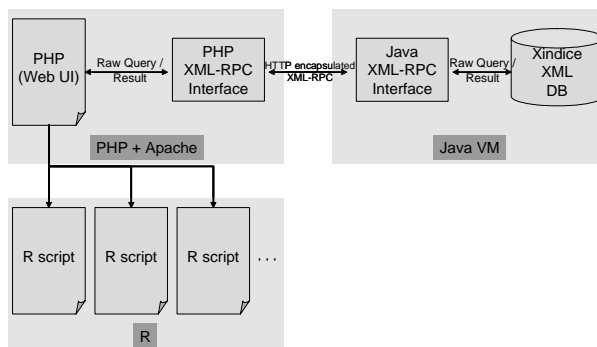


Figure 1: Diagram of the workbench system

PHP scripting language [2] is used for implementation of web-based user interface. All data, such as user account, quantification data and calibration information, is stored in Xindice XML database. XML-RPC [3] protocol is used for communication between PHP application and Xindice. R language [4] is utilized for multivariate analysis and visualization, such as principal component analysis (PCA) and hierarchal cluster analysis.

3 Conclusion

We developed a workbench system for quantification and multivariate analysis of phospholipids. Screenshots of the system are shown in Figure 2.

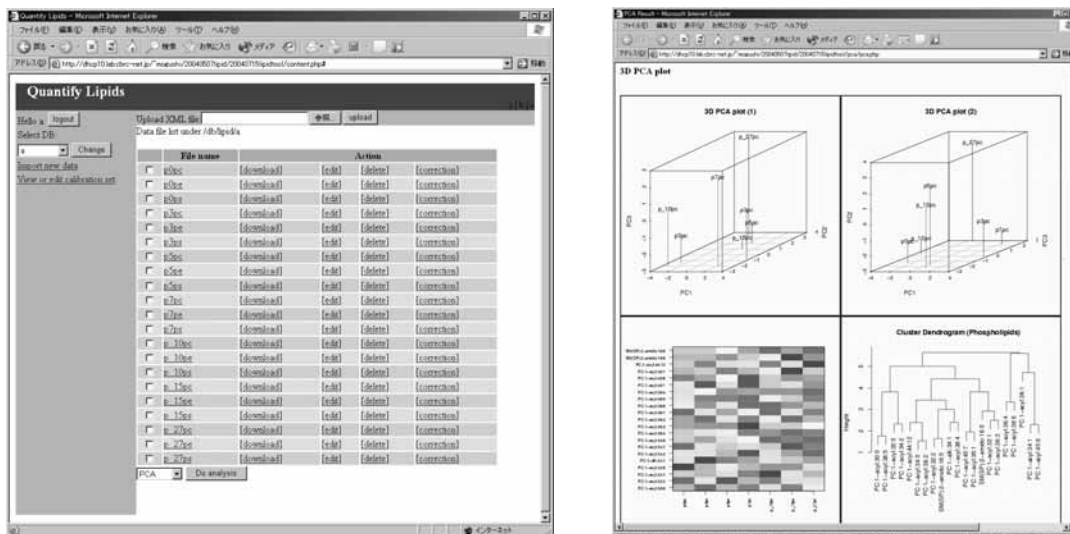


Figure 2: Screenshots of the workbench system.

Left: List view of experiment data. Right: Example of PCA and hierarchal clustering analysis.

References

- [1] <http://xml.apache.org/xindice/>
- [2] <http://www.php.net/>
- [3] <http://www.xmlrpc.com/>
- [4] <http://www.r-project.org/>