omics.data.edu.au

Metabolomics Requirements Summary

This document is a high level summary of the Metabolomics area requirements and information captured during the discoverability phase of the RDS Omics project

Summary

Metabolomics is the scientific study of chemical processes involving metabolites. Specifically, metabolomics is the "systematic study of the unique chemical fingerprints that specific cellular processes leave behind", the study of their small-molecule metabolite profiles.The metabolome represents the collection of all metabolites in a biological cell, tissue, organ or organism, which are the end products of cellular processes. mRNA gene expression data and proteomic analyses reveal the set of gene products being produced in the cell, data that represents one aspect of cellular function. Conversely, metabolic profiling can give an instantaneous snapshot of the physiology of that cell. One of the challenges of system biology and functional genomics is to integrate genomic, proteomic, transcriptomic and metabolomic information to provide a better understanding of cellular biology.

Groups Consulted

Metabolomics Australia at Bio21, the University of Melbourne

Work Pattern

Acquisitions are managed via the MASTR-MS laboratory information management system which holds relevant information and acquisition details for each project. The acquisitional sequence list is transferred to the instruments and utilised to make the acquisition. Raw data is returned to MASTR-MS. Facility staff access the raw data and analyse it with XCMS via methods that are tailored to the scientific goals of the project. The end products are a spreadsheet and a summary powerpoint.

Data Overview

The raw data in Agilent “.D” format
The processed data in a CSV file

Software/Applications used

- XCMS (see https://metlin.scripps.edu/xcms/)
- Metabolomics Australia R

Deficiencies in processes and tools

Data are not yet provided via BPA repository. Users generally don't access raw data, they receive the CSV files via email. The OMICS platform will need both raw and processed data.

Scale of Data

It is expected that in total about 500 samples would be run for the BPA Sepsis project. Each of these runs would produce a raw data file (size approximating 50MB) and a processed data file (CSV format, size approximating 10 MB max).

Relationship with other Streams

Since Metabolomics is the downstream omics of the omics pipeline, the experimental design and analysis of results does not depend on the outcome of the other omics' results. Having said that, once all the data is collected, one can scrutinize a selected set of metabolites and their role in pathways based on any interesting observation made in the other omics. Conversely, if a certain pathway was highlighted in the metabolomics analysis, this information can be used to selectively query data of other omics.