Biomarker detection in LC-MALDI mass spectrometry proteomic profiles using R

Grégoire R. Thomas, Sven Degroeve, Koen De Cremer, Filip D'Hondt, Koen Kas, Luc Krols

PEAKADILLY nv, Technologiepark 4, VIB Bio-Incubator, B-9052 Zwijnaarde/Ghent – Belgium

http://www.peakadilly.com/

Reliable biomarker discovery has a dramatic impact on current and future healthcare. Peakadilly's unique proteomics platform allows biomarker discovery in the context of different biological and clinical problems and different biological samples, with an emphasis on serum biomarker discovery.

Peakadilly here describes the robust analysis of LC-MALDI MS data for the discovery of clinical biomarkers using R (http://www.r-project.org/). The biological samples are analysed using COFRADIC™, a powerful gel-free proteomics technology (Nat Biotechnol. 21:566-9, 2003). COFRADIC™ reduces the complexity of an enzymatic digest without loosing information on protein content. This allows sensitive proteome-wide profiling of complex biological and clinical samples.

For each biological sample, a COFRADIC™ analysis generates several hundred spectra each corresponding to an elution fraction from the LC system. The resulting LC-MS profiles are intensity maps representing the expression levels of proteins.

Peakadilly's biomarker discovery pipeline comprises visualisation of LC-MS profiles, feature detection, alignment of the different LC-MS profiles, generation of expression matrices, integration of tandem MS data, and data-mining. The analysis pipelines generates expression matrices derived from thousands of proteins. Candidate biomarkers are extracted by selecting the features that are differentially expressed between groups of samples.

Abbreviations: MS, mass spectrometry; LC, liquid chomatography; MALDI, matrix-assisted laser desorption/ionisation