A Complete Solution for Targeted Lipid Analysis using a Smart Compact LC-ToF

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Introduction

Routine lipid analysis can be performed once a potential biological marker of disease has been hypothesized and identified using advanced mass spectrometry techniques such as ion mobility or SONAR acquisitions. Assays looking for the identified targets or for class changes, can be performed to test the validity of the biomedical hypothesis.

The ACQUITY™ RDa Detector is able to simplify analysis of complex samples compared to traditional Q-ToFs. Acquiring data for a high number of analytes without suffering from small dwell times or missing important components due to quadrupole selection experienced using triple quadrupole instruments.

Experimental

Plasma precipitated with ice cold IPA.

Supernatant was analysed on an ACQUITY RDa Detector in ESI+

Separation via a typical UPLC RP gradient.

Data was acquired and processed with UNIFI™ software and statistical analysis performed with MetaboAnalyst 5.0.software.

Results

Robustness data was processed within UNIFI software using curated .mol file libraries.

MetaboAnalyst was used for Multivariate statistical analysis.

Robustness over a >6 days analysis time:

- Demonstrated an average mass accuracy deviation of ±2.0 ppm
- Showed an average 5.2%.peak response deviation.
- Chromatographic retention time varied <5 seconds over the entire analysis.

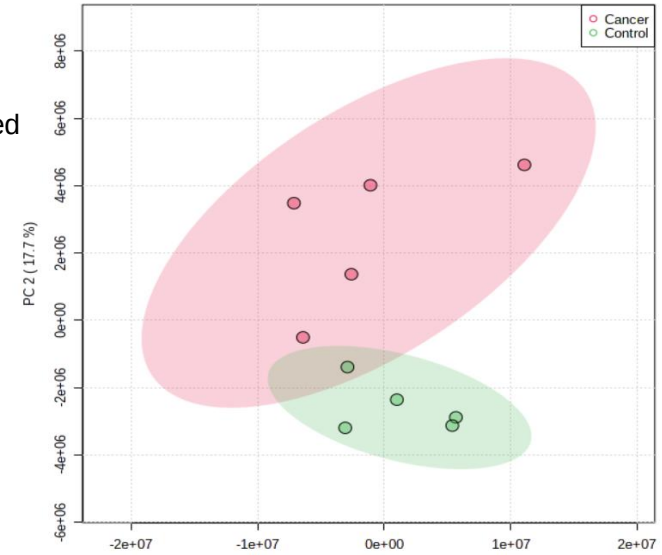

Figure 2: A lung cancer vs healthy control sample set, demonstrating a standard workflow importing the data into Metaboanalyst.

Data displayed: unsupervised PCA plot with no data scaling or normalization.

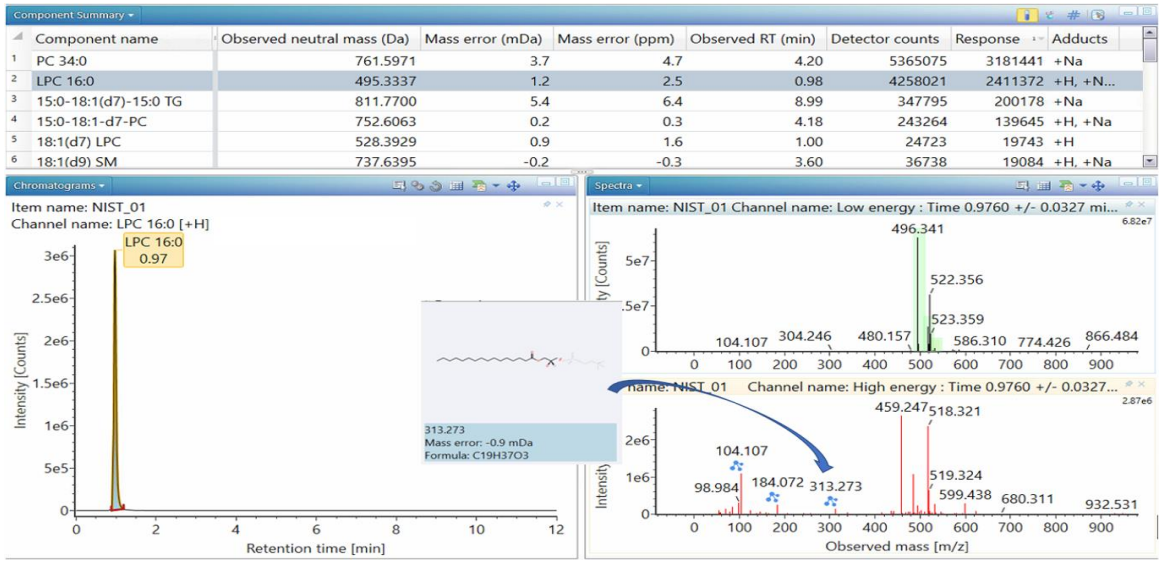

Figure 1: UNIFI display showing table of identifications for one selected injection

Conclusions

The ACQUITY RDa Detector provides a robust platform for simple, routine screening for known lipids using a library database. It is well suited to known target analysis applications by less experienced mass spectrometer users. Maintaining excellent data consistency and mass accuracy.

Data can be easily exported to alternative processing and statistical software packages such as MassLynx, Progenesis™ QI, or converted to an mzML file format.