

Comparing Nontargeted LC-MS Methods by Co-Visualizing Linear Range and Chemical Coverage

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Introduction

Background

Nontargeted LC-MS results strongly depend on instrumental setup.

Challenge

How to compare nontargeted methods systematically? What criteria to use for method optimization?

Example

Evaluation of high-temperature vs. standard-temperature electrospray ionization (Fig. 1)

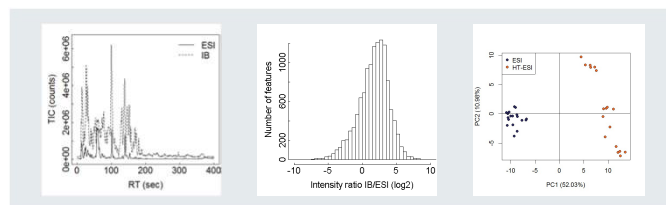
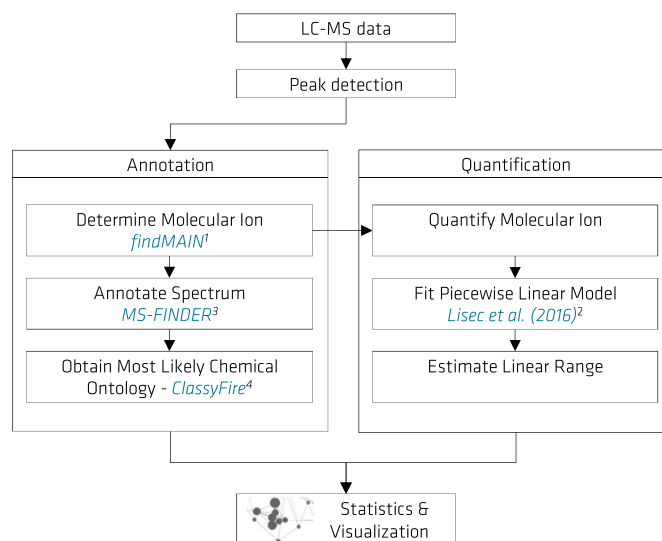


Fig. 1: Dependency of metabolomic fingerprints on ion source used. A high-temperature source (Bruker IonBooster, IB), typically operated at 400°C, was compared to standard ESI interface (ESI) typically operated at 200°C. Left: Total ion currents (TIC) demonstrating differences in overall sensitivity. (B) Distribution of feature intensity ratios IB vs. ESI. (C) PCA scores for the same (lipidomics) samples acquired on both ion sources.

Methods

Approach

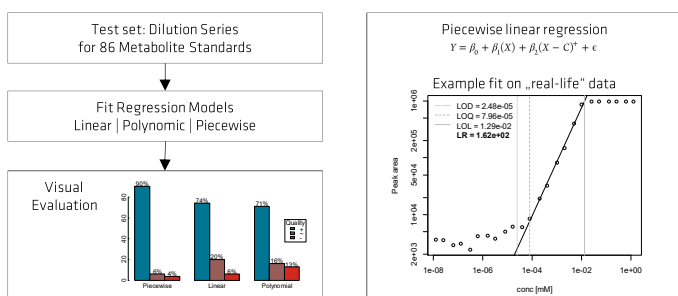
Evaluating linear range and chemical class for all features, using an automated R workflow



Results

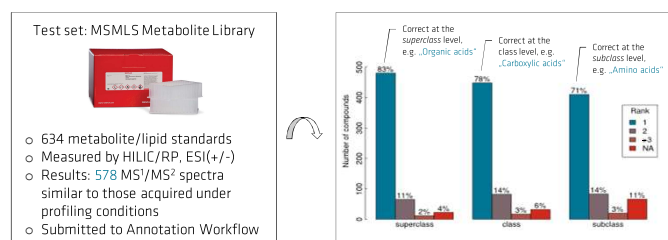
Validation (1): Unsupervised linear range determination

→ Piecewise linear regression performed the most robustly



Validation (2): Unsupervised chemical classification

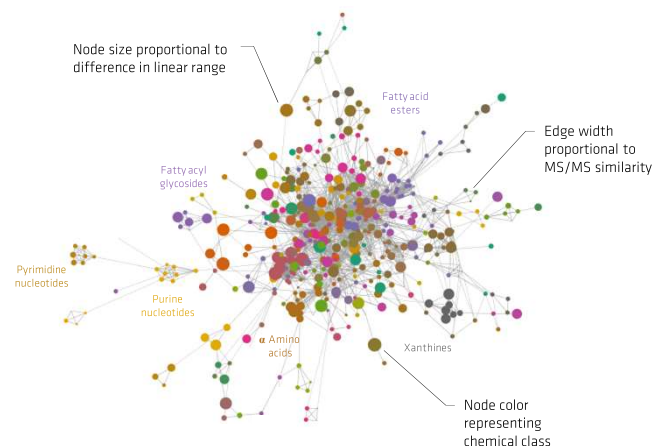
→ 83% accuracy achieved for a chemically diverse test set



References

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- Lisec J, Hoffmann F, Schmitt C, Jaeger C (2016). *Anal. Chem.* DOI: 10.1021/acs.analchem.6b02515
- Tsugawa H, Kind T, Fiehn O, Arita M et al. (2016). *Anal. Chem.* DOI: 10.1021/acs.analchem.6b00770
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Putting it together: Co-visualizing linear range and chemical coverage on a molecular network



- Analysis reveals potential differences in selectivity between two nontargeted methods
- Here: Comparison of high-temperature (HT) vs. standard-temperature (ST) ESI revealed differences mainly regarding amine compounds

