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)

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

Putting it together: Co-visualizing linear range and chemical coverage on a molecular network

References