044: A New Generation of Reference Materials to Promote High Quality Data in Untargeted Metabolomics

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Why?

- Urgent need to increase data accuracy and reproducibility
- Distinguish experimental variance from systematic error
- Harmonize across protocols, analysts, instruments, and laboratories
- More economical RMs with accelerated development

How?

- Qualitative characterization of metabolite profiles
- Measured using multiple platforms
- Highly confident annotations

Liquid chromatography – tandem mass spectrometry

NMR spectroscopy

What do plasma, urine, liver and feces have in common?

NIST is creating these as reference materials for use in your **untargeted metabolomics studies**

What?

NIST Reference Materials (RM): non-certified, informational values; sufficiently homogeneous and stable materials

- The materials are suites with multiple phenotypes:
  - RM 8231 Frozen Human Plasma Suite (high TG, diabetic, young African American)
  - RM 8232 Frozen Human Urine Suite (smoker, non-smoker, male/female)
  - RM 8462 Frozen Human Liver Suite (normal, fatty, congested)
  - RM 8048 Human Fecal Material (omnivore and vegetarian)
- Unified multi-platform, multi-method, multi-algorithm QA/QC tools
- Associated reference data containing list of annotated metabolites
- Distinct profiles for application in differential analysis
- Broad characterization of complex materials to match specific matrices

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Differential Analysis Example

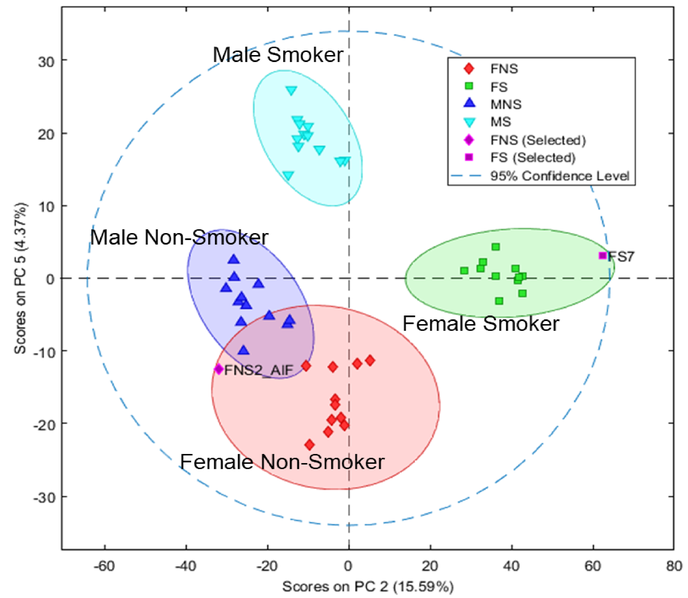

Figure 1. RM 8232 principal component analysis demonstrating separation between material phenotypes

Annotation Method Example

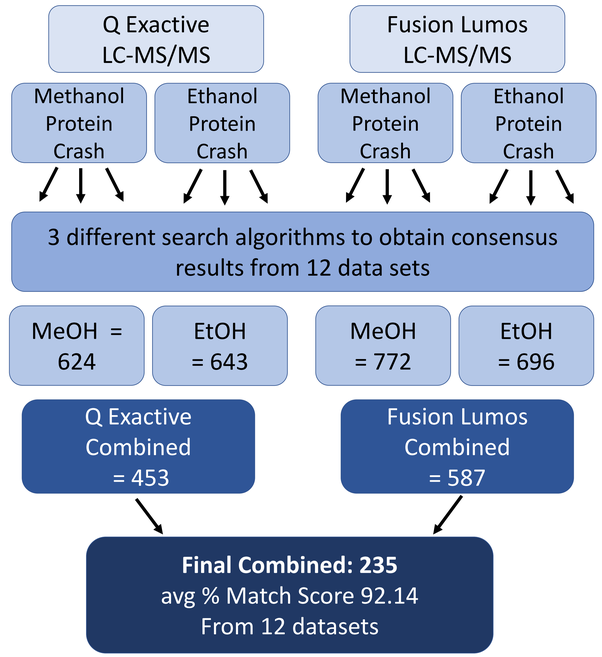

Figure 2. Workflow with final number of confident annotations in RM 8231 Type 2 Diabetic Plasma