



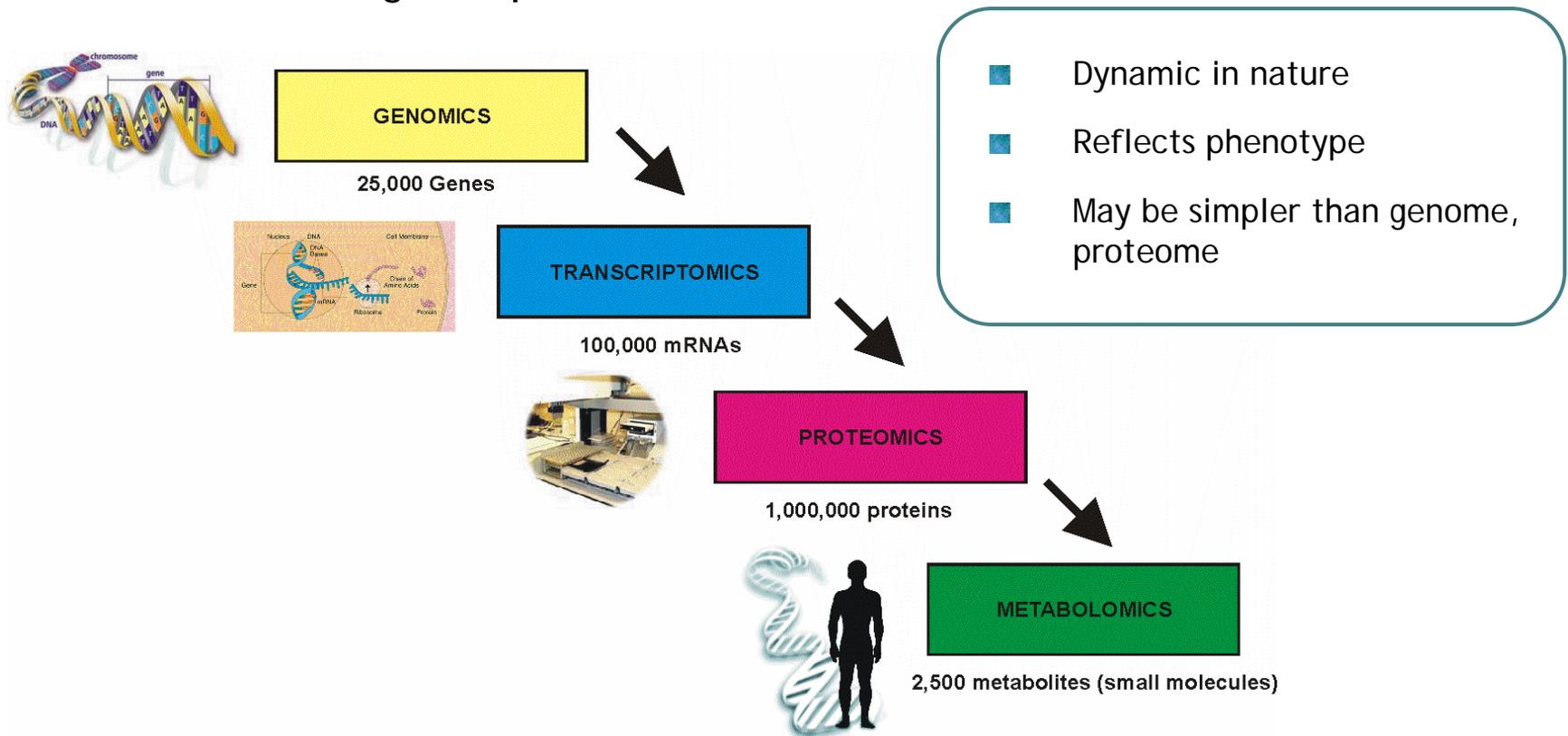
# Standards Development for Metabolomics

Karen W. Phinney

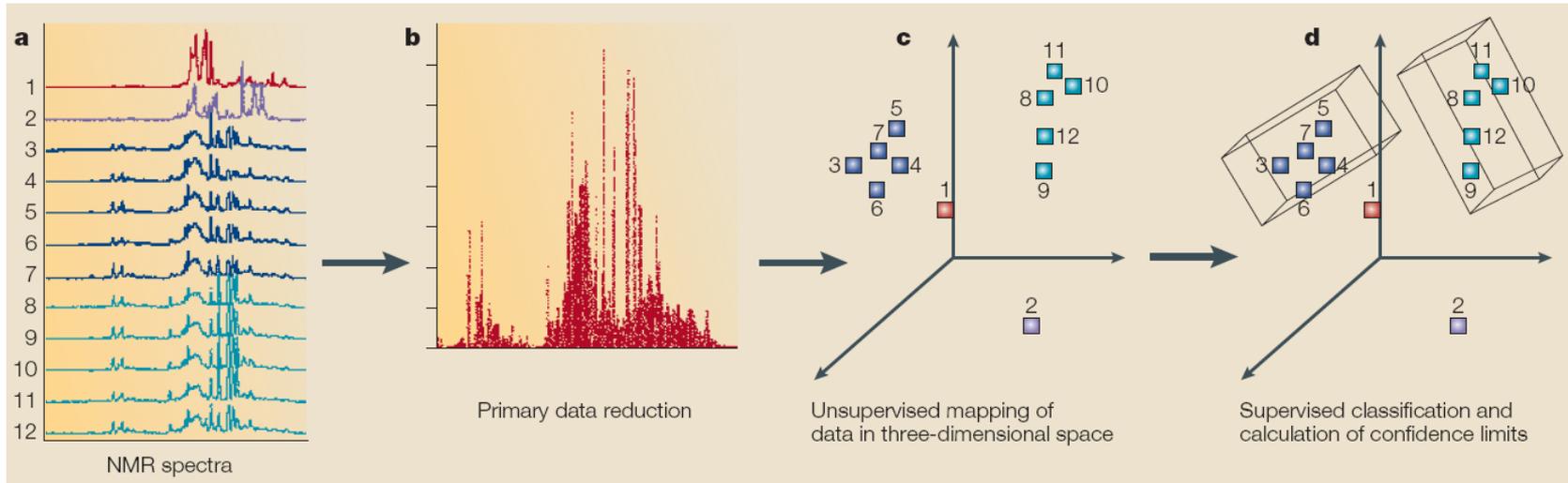
Analytical Chemistry Division, Chemical Science and Technology  
Laboratory, National Institute of Standards and Technology

# Metabolomics

The **metabolome** represents the identity and concentration of metabolites at a given point in time



# Goals of Metabolomics

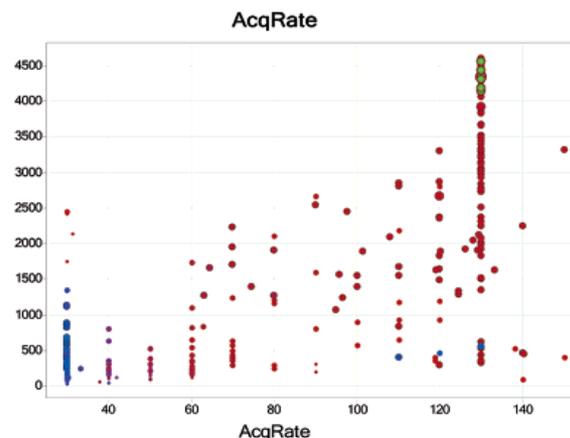


Nicholson et al., 2008

- Identification of new diagnostic tools
- Therapeutic targets (metabolic pathways)
- Drug toxicity
- Studies of gene function

# What Are the Issues?

- Comparison of different data sets
  - Sampling
  - Instrument variations
  - Software
- Identification of statistically significant metabolites
  - Data deconvolution
  - Spectral databases
- Validation of metabolites



Kell et al., 2007

# Reference Material Design - SRM 1950

- New SRM 1950 Metabolites in Human Plasma is being developed to provide a well-characterized reference material for metabolomics technology development
- Plasma samples collected from approximately 100 individuals
- Equal number of healthy men and women, 40 - 50 years of age
- Racial distribution similar to that of U.S. population
- Total plasma volume ~ 20 L
- Both quantitative and qualitative (identity) information



# Additional Needs

- Control samples for specific populations and matrices
- Tools for data alignment of complex data sets
- Validation of statistical models for pattern recognition
- Reporting standards - Metabolomics Standards Initiative

