



Metabolite Identification

**Tools & Methods for MS
Metabolomics in Nutrition**

Claremont-Ferrand, Dec. 12, 2007

David Wishart, University of Alberta

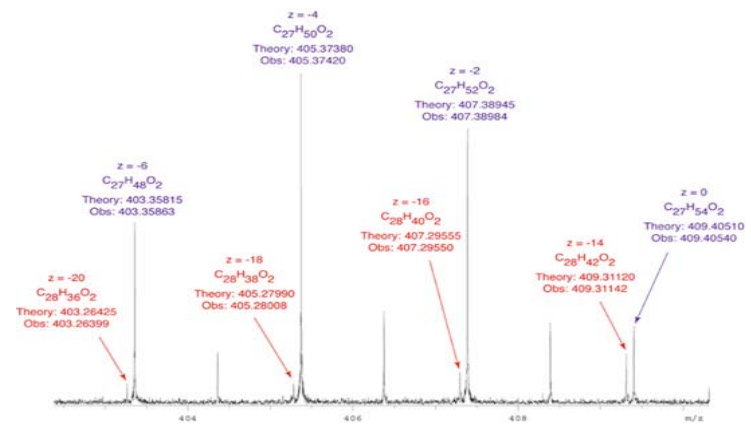
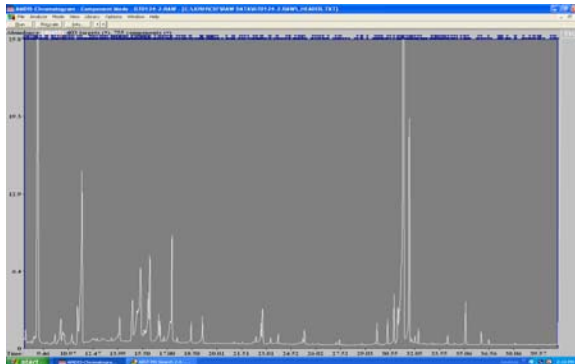
Workshop Summary

- **Sampling, Storing & Processing**
 - Lorraine Brennan
- **Mass Spectrometry Analyses**
 - Thomas Hankemeier
- **Data Extraction**
 - Elwin Verheij
- **Data Analysis**
 - Bruce Kristal
- **Metabolite Identification (Dec. 14, 9:30-12:00)**
 - David Wishart
- **Biological Interpretation**
 - Suzan Wopereis & Ben Van Ommen

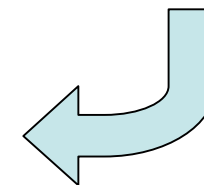
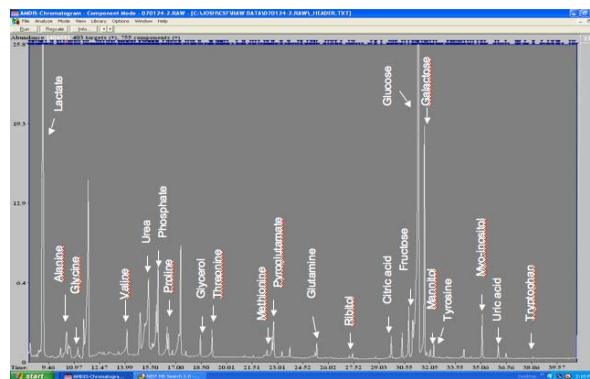
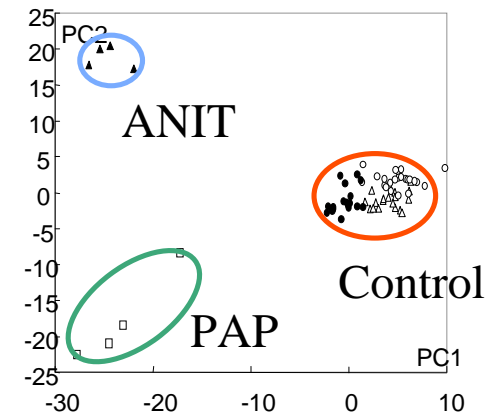
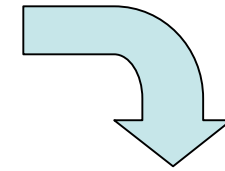
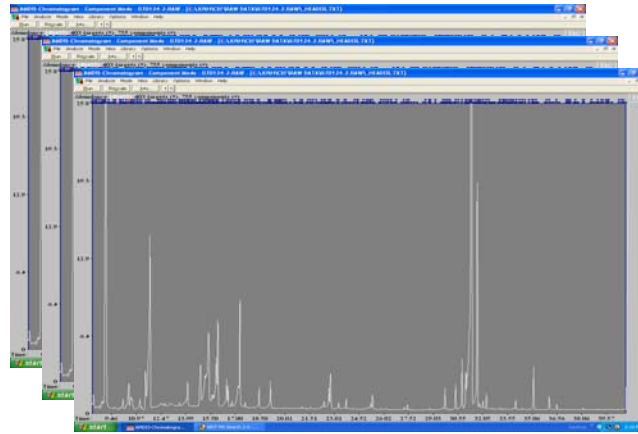
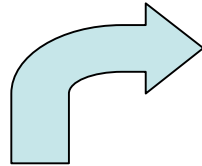
Separation Technologies



MS Technologies

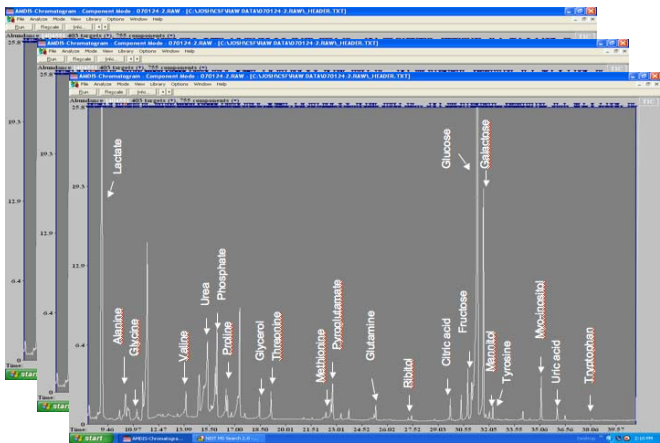
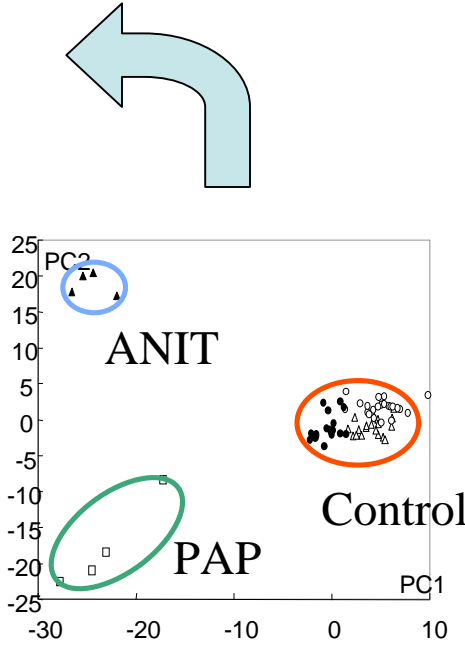
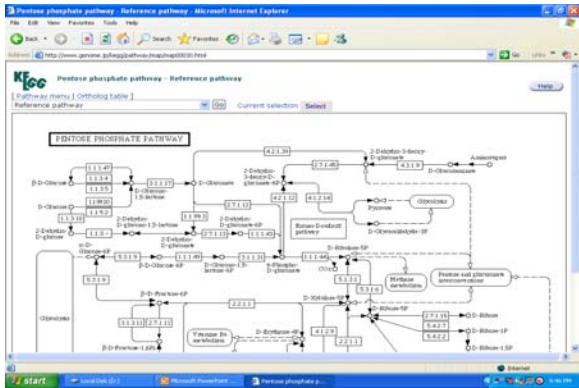


Two Routes to Metabolomics



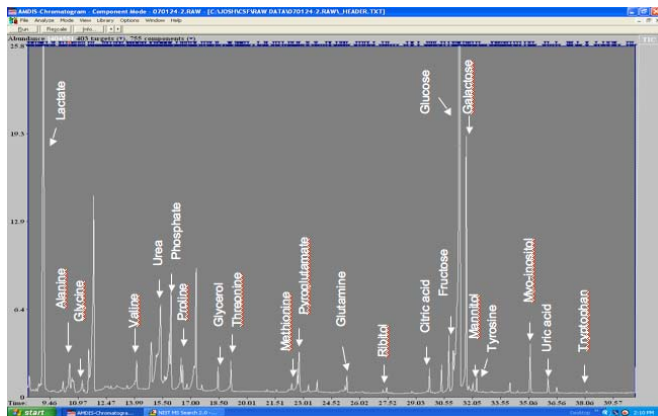
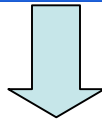
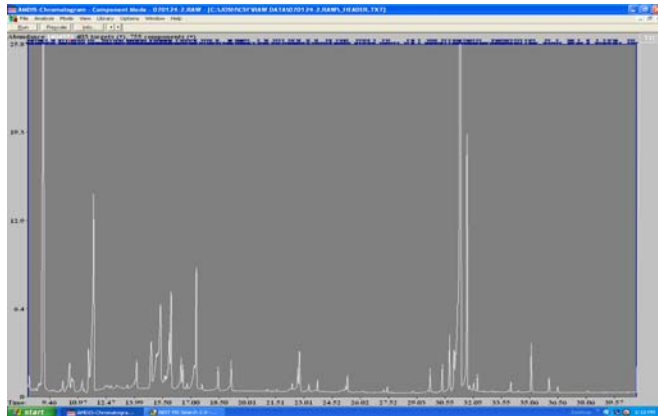
Metabolite Identification

Two Routes to Metabolomics



Metabolite Identification

Metabolite Identification



- Analyze EI or MS/MS fragmentation patterns
- Verify with authentic standards
- Search through MS databases
- Determine molecular formula from exact mass
- Perform NMR studies on purified compound
- Supplement with IR or UV information
- Perform chemical tests on purified compound

De novo vs. known

Workshop Goals

- **Exchange knowledge and experience in metabolite identification strategies for GC-MS, LC-MS and other MS-based techniques**
- **Come up with methods or protocols to increase the number and reliability of identified/quantified metabolites in common matrices in nutritional metabolomic studies**

Workshop Topics

- **Additional topics are always welcome**
- **GC-MS databases**
 - What is needed to make them relevant to metabolomics and biomarker profiling?
- **GCxGC-MS databases**
 - How to prepare appropriate databases and search tools for metabolite identification and quantification?

Workshop Topics

- **Reference Compound libraries**
 - What is available and how should these be maintained?
- **LC-MS and LC-MS/MS databases**
 - What kinds of information need to be captured/displayed to make them useful?
- **CE-MS and LC-IMS-MS**
 - Can/should spectral databases for these technologies be established?

Workshop Topics

- **Quantification of metabolite data by MS**
 - How to do it?
- **Automated compound ID by GC/LC MS**
 - How can spectral databases play a role?
- **Defining biomarkers**
 - Is one compound enough? Are multiple compounds required? How to define a robust biomarker profile?

Workshop Topics

- **Can/should biofluid or biomarker profiles be databased?**
- **Can/should raw LC-MS and GC-MS spectra be databased?**
- **What is the role of private/public spectral databases?**
- **What is the role of private/public software in metabolite ID?**

Workshop Topics

- **What kind of data exchange format or data submission standards be used to create MS databases?**
- **What kind of data needs to be in these databases?**
- **Should a common, public, metabolomic specific MS database (GenBank) be created? If so, how and by whom?**

Workshop Topics

- Do we need to establish or create “gold standards” or special “testing mixtures” to assess metabolite ID and quantification by different MS methods or different MS labs?
- Will testing standards improve reliability and reproducibility?
- Anything else?

Metabolite ID Reminder

- **Friday Dec. 14**
- **9:30 am - 12:00 noon**
- **Parallel session with “Data Analysis”**
- **Summary session 1:30 - 2:00 pm**

- **Thanks to... Augustin Scalbert, Jane Hubert, Claudine Manach, Jean-Francois Martin, Estelle Pulos, Jean-Louis Sebedio, Ivan Bobeldjik-Pastorova, Suzan Wopereis, TNO & INRA**