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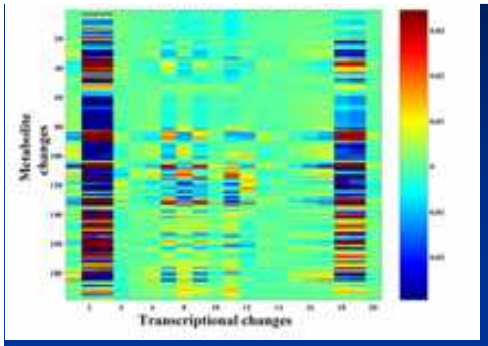
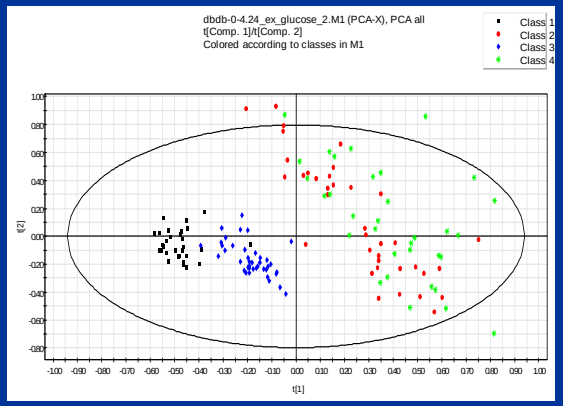


Presentation by the Metabolomics Society Committee on Standardisation

Jules Griffin, Cambridge



Aim

- To give an overview of the current level of discussions in terms of the standardisation of reporting metabolomic data.
- To recruit interested parties.

Introduction to the Metabolomics Society Committee on Standardisation

- In analogy to proteomic or transcriptomic experiments, a great richness in data is acquired in global metabolic studies.
- Potentially, such data could be re-used by other researchers using different bioinformatics or chemometric techniques.
- However, without establishment of a common ontology and structure how metabolomic data should be reported, comparisons will not be possible despite the willingness of most researchers to report details on experimental procedures and other metadata.

- A number of efforts have been attempted in standardizing reporting structures:
  - Lindon J.C. *et al.* Nat. Biotechnol. 2005, 23, 833-838 ,
  - Jenkins H. *et al.* Nat. Biotechnol. 2004, 22, 1601-1605)
  - MetaboMeeting 1.0 in Cambridge, UK July 2005, U.K.
  - The Metabolomics Standards workshop hosted by the NIH/NIDDK in Bethesda, USA, Aug 2005.
- Resulting from these efforts were agreements to write a draft document on 'Reporting standards in Metabolomics'

Scope

- The scope of these efforts will be to identify, develop and disseminate best practice in all aspects of metabolomics.
- The aim will not be to ***prescribe*** how to do metabolomics experiments but to formulate a minimum of reporting standards that ***describe*** the experiments.
- Consequently, there will be no attempt to restrict or dictate specific practices but to develop better descriptors to support the dissemination and re-use of metabolomic data.
- Such reporting standards will specify the data identified as necessary for complete and comprehensive reporting in a range of identified contexts, such as submission to academic journals.

Oversight committee

- The Metabolomics Society appointed an oversight committee chaired by Oliver Fiehn (ofiehn@ucdavis.edu) with members Rima Kaddurah-Daouk, Susanna Sansone, Pedro Mendes, Bruce Kristal, Nigel Hardy, Lloyd Sumner, Ben Ommen, John Lindon, and, ex-officio, John Quakenbush and Arthur Castle.
- **The oversight committee has identified five areas of utmost importance for describing metabolomic experiments:**
  A. Biological sample context
- Interim Overall Chair: Don Robertson — Donald.Robertson@pfizer.com
  subchair: 'in vivo / mammalian biology': — joint chairs Jules Griffin jlg40@mole.bio.cam.ac.uk and Wayne Matson Wane.Matson@va.gov
  subchair 'plant biology': — Basil Nikolau dimmas@iastate.edu
  subchair 'in vitro / cell culture biology': — Mariet van der Werf vanderWerf@voeding.tno.nl
  subchair 'environmental analysis': — Norman Morrison Norman.Morrison@manchester.ac.uk
  B. Chemical analysis
- Interim joint chairs: — Lloyd Sumner lwsumner@noble.org and Teresa Fan teresa.fan@louisville.ed
- **C. Data analysis**
- Interim Chair: — Roy Goodacre roy.goodacre@manchester.ac.uk
- **D. Ontology**
  Interim Chair: — Susanna-Assunta Sansone sansone@ebi.ac.uk
  E. Data Exchange
  Interim Joint Chairs: — Nigel Hardy nwh@aber.ac.uk and Chris Taylor chris.taylor@ebi.ac.uk

- Each group will :
- work cooperatively on a consensus draft for a minimum core set of necessary data for their specialist area
- include key persons from the group's specialist area to take part in the discussion in an inclusive manner.
- reach out and evaluate to previous and relevant work in their specialist areas including similar work in transcriptomics and proteomics studies, and recent metabolomics standardization efforts.
- pay careful attention to the distinction of best practice (which will change), reporting standards (which should have longer validity) and data exchange standards (which support reporting).
- respond to documents from the other groups and produce an advanced draft ready for discussion in February 2006
- respond to documents from the other groups and produce a final draft ready for discussion in June 2006

Standardization in Metabolomics
Biology Subcommittee Teleconference

- Still meeting at the chair/sub-chair level via teleconferences
- A. Participants reviewed several currently operating standardization efforts that have or may have applicability towards our efforts in metabolomics.
  - SMRS, ARMET, MIAME, RSBI, FUGO, MIGS, MIAPE, CEBS
- Based on the discussion, it was concluded to focus further efforts on 3 approaches.
  - MIGS,
  - MIAME
  - CEBS.
  - Other initiatives have good representation on the committee (or plans were to make contact)
- All participants agreed to review relevant documentation provided by the rapporteurs with special emphasis on how the described standardization effort would harmonize (or not) with each member's particular subcommittee.
  - For example, how will plant or bacterial data and definitions mesh with terms and definition in the CEBS dictionary?

MIGS

- MIGS – Minimum Information about Genomic Sequences
- What were it's original aims?
  - The development of a new standard to capture a richer set of information describing complete genomes
- Parts, such as sample, environment and phenotype description are synergistic with other efforts.

MIAME

- MIAME describes the Minimum Information About a Microarray Experiment that is needed to enable the interpretation of the results of the experiment unambiguously and potentially to reproduce the experiment. They have also achieved the adoption of this as a requirement for publication for a number of journals.
- The intention is to extend this initiative to other functional genomic technologies.
- This initiative has a large audience.
  - The website has a bite sized version of the description!

CEBS

- CEBS is a public toxicogenomics database, defining toxicogenomics broadly to include transcriptomics, protoemics, metabolomics, genomics data in the context of toxicology, pharmacology, environmental health, etc.
- The original audience includes interested members of the public (e.g. one-off queries), researchers interested in comparing their private data with public data, and people interested in using biological endpoint data (pathology, clin chem., etc) to query toxicogenomics data.

Next steps

- **Face to Face Meeting**
  - Aim for May 2006 at the committee and sub-committee level
  - Draft biology context recommendations by May 2006.
  - Presentation of the recommendations at the Metabolomics Society meeting in June.
- **Begin to populate the sub-committees**
  - We would like to recruit interested parties

One final thought…

- This is an open initiative and the success depends on the breadth of engagement. Please, contact the appropriate interim chair if you are willing to help with your expertise to the standards development process.