

Standardization in Metabolomics Experiments:

A discussion forum of the Metabolomics Society for drafting a document on best practice, reporting and data exchange

Comprehensive analysis of metabolic responses (Metabolomics and Metabonomics) has been made possible and useful with the advent of modern computational and analytical tools in the 1990's. In conjunction with sequenced genomes and online access to a wealth of medical and biological information, today metabolomics is applied to both clinical trials and fundamental research.

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, standards are lacking that guide researchers to report in detail how data were actually acquired, which experimental designs were used, and how data were processed and structured to eventually reason scientific conclusions. Furthermore, the flexibility of metabolism and the need for validation of disease biomarkers or biochemical events across different diseases requires comparison of different metabolomic datasets between laboratories and beyond specific techniques. However, without establishment of a common ontology and structure how metabolomic data should be reported, comparisons will be disabled despite the willingness of most researchers to report details on experimental procedures and other metadata.

Therefore, metabolomic researchers have undertaken great efforts in standardizing reporting structures culminating in two larger research papers (Lindon J.C. *et al.* Nat. Biotechnol. 2005, 23, 833-838, Jenkins H. *et al.* Nat. Biotechnol. 2004, 22, 1601-1605) and two discussion conferences in summer 2005, [MetaboMeeting 1.0](#) in Cambridge, U.K. and the [Metabolomics Standards workshop](#) hosted by the NIH/NIDDK in Bethesda, USA.

Resulting from these efforts were agreements to write a draft document on 'Reporting standards in Metabolomics' that aims at reaching a consensus and that might therefore serve as guideline for researchers, journals, funding and scientific organizations, vendors and regulatory bodies.

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. Data exchange standards will be developed to provide a technical vehicle which meets or exceeds the requirements of reporting standards.

Working groups

The Metabolomics Society has appointed an oversight committee to monitor, coordinate and review the efforts of working groups in specialist areas that will examine standardization and make recommendations before June 2006. This oversight committee is 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	lwsunner@noble.org
	and Teresa Fan	teresa.fan@louisville.ed

C. Data analysis

Interim Chair:	Roy Goodacre	roy.goodacre@manchester.ac.uk
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D. Ontology

Interim Chair:	Susanna-Assunta Sansone	sansone@ebi.ac.uk
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E. Data Exchange

Interim Joint Chairs:	Nigel Hardy	nwh@aber.ac.uk
	and Chris Taylor	chris.taylor@ebi.ac.uk

Each group will :

1. work cooperatively on a consensus draft for a minimum core set of necessary data for their specialist area
2. include key persons from the group's specialist area to take part in the discussion in an inclusive manner.
3. 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.
4. 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).
5. respond to documents from the other groups and produce an advanced draft ready for discussion in February 2006
6. respond to documents from the other groups and produce a final draft ready for discussion in June 2006

For each group, the work will be coordinated by the group's chairpersons using email, shared documents and telephone conferences which will be organized with the help of the Metabolomics Society.

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.

For the oversight committee: Oliver Fiehn, UC Davis

October 10, 2005