# CIMR: Plant Biology Context

Metabolomics Standards Initiative (MSI)


**Sponsor:** Metabolomics Society http://www.metabolomicssociety.org/

**Reference:** http://msi-workgroups.sourceforge.net/bio-metadata/reporting/pbc/

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**Authors:** Basil Nikolau, Iowa State University <dimmas@iastate.edu>
Oliver Fiehn, UC Davis, CA <ofiehn@ucdavis.edu>
the participants of the 2006 Plant Metabolomics Conference and:
Sue Rhee, TAIR <rhee@acoma.Stanford.EDU>
Julie Dickerson, Iowa State University <julied@iastate.edu>
Mark Lange, Washington State University <lange-m@wsu.edu>
Geoff Lane, AgResearch, New Zealand. <geoff.lane@agresearch.co.nz>
Ute Roessner, University of Melbourne, Australia
<ute.roessner@acpfg.com.au>
Jane Ward, Rothamsted Research, England <jane.ward@bbsrc.ac.uk>
Robert Last, Michigan State University <lastr@msu.edu>
Clint Chapple, Purdue University <chapple@purdue.edu>
Edited by Nigel Hardy

**Credits:** *Chair*: Basil Nikolau




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# 1. This document

This document forms part of the the standards for reporting metabolomics experiments developed under the Metabolomics Society (http://www.metabolomicssociety.org/Metabolomics Standards Initiative (MSI). It should be read in the context of top level document for those standards [1] .

The current version of the document is work in progress. ???.

# 2. Scope and Goals

## 2.1. Scope of the Plant Biological Context subgroup

The scope of our efforts will be to identify, develop and disseminate best reporting practices in all

aspects of plant metabolomics that are related to describing the plant biology experimental designs. The proposed standards will be consistent with good plant biology practices with extra provisions for the need to be able to compare experimental designs electronically, and will be in alignment with those typically required by quality analytical journals.

The aim will not be to *prescribe* how to perform a plant metabolomics experiments, but to formulate a minimum set of reporting standards that *describe* the experiments (what are the experiments and how they were actually executed). Consequently, there will be no attempt to restrict or dictate specific practices, but to develop consistent and appropriate 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 and public databases. Data exchange standards will be developed to provide a transparent technical vehicle which meets or exceeds the requirements of reporting standards.

## 2.2. The Goals of the Plant Biology Context Group

1. To work cooperatively on a consensus draft for a *minimum core set* of necessary metadata needed to understand, repeat, compare and re-investigate metabolomic data resulting from the plant experimental design with respect to physiological, morphological and genetic aspects.
2. To include key persons from the field of plant biology to participate in the discussion in an inclusive manner.
3. To reach out and evaluate previous and relevant work in plant biology including similar work in transcriptomics and proteomics studies, and recent metabolomics standardization efforts.
4. To 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. To respond to documents from the other groups and produce an advanced draft ready for discussion in June 2006

# 3. Related Work

## 3.1. Related literature

[1] Bino, R. J. and Hall, R. D. and Fiehn, O. and Kopka, J. and Saito, K. and Draper, J. and Nikolau, B. J. and Mendes, P. and Roessner-Tunali, U. and Beale, M. H. and Trethewey, R. N. and Lange, B. M. and Wurtele, E. S. and Sumner, L. W.. *Potential of metabolomics as a functional genomics tool*. *Trends In Plant Science*. 9. 9. 418-425. 2004.

[2] Jenkins, H. and Hardy, N. and Beckmann, M. and Draper, J. and Smith, A. R. and Taylor, J. and Fiehn, O. and Goodacre, R. and Bino, R. J. and Hall, R. and Kopka, J. and Lane, G. A. and Lange, B. M. and Liu, J. R. and Mendes, P. and Nikolau, B. J. and Oliver, S. G. and Paton, N. W. and Rhee, S. and Roessner-Tunali, U. and Saito, K. and Smedsgaard, J. and Sumner, L. W. and Wang, T. and Walsh, S. and Wurtele, E. S. and Kell, D. B.. *A proposed framework for the description of plant metabolomics experiments and their results*. *Nature Biotechnology*. 22. 12. 1601-1606. 2004.

[3] Jenkins, Helen and Johnson, Helen and Kular, Baldeep and Wang, Trevor and Hardy, Nigel. *Toward Supportive Data Collection Tools for Plant Metabolomics*. *Plant Physiol. %R 10.1104/pp.104.058875*. 138. 1. 67-77. 2005.

[4] Lindon, J. C. and Nicholson, J. K. and Holmes, E. and Keun, H. C. and Craig, A. and Pearce, J. T. M. and Bruce, S. J. and Hardy, N. and Sansone, S. A. and Antti, H. and Jonsson, P. and Daykin, C. and Navarange, M. and Beger, R. D. and Verheij, E. R. and Amberg, A. and Baunsgaard, D. and Cantor, G. H. and Lehman-McKeeman, L. and Earll, M. and Wold, S. and Johansson, E. and Haselden, J. N. and Kramer, K. and Thomas, C. and Lindberg, J. and Schuppe-Koistinen, I. and Wilson, I. D. and Reily, M. D. and Robertson, D. G. and Senn, H. and Krotzky, A. and Kochhar, S. and Powell, J. and van der Ouderaa, F. and Plumb, R. and Schaefer, H. and Spraul, M.. *Summary recommendations for standardization and reporting of metabolic analyses*. *Nature Biotechnology*. 23. 7. 833-838. 2005.

[5] Orchard, S. and Hermjakob, H. and Apweiler, R.. *The proteomics standards initiative*. *Proteomics*. 3. 7. 1374-1376. 2003.

[6] Orchard, Sandra and Hermjakob, Henning and Taylor, Chris and Aebersold, Ruedi and Apweiler, Rolf. *Human Proteome Organisation Proteomics Standards Initiative Pre-Congress Initiative*. *PROTEOMICS*. 5. 18. 4651-4652. 2005.

[7] Quackenbush, John. *Data standards for 'omic' science*. 22. 5. 613. 2004.

## 3.2. Related Internet Sites

http://www.smrsgroup.org/
http://www.niddk.nih.gov/fund/other/metabolomics2005/
http://www.metabolomicssociety.org/nih.html
http://www.mged.org/Mission/index.html#DefinedMGEDStandards
http://psidev.sourceforge.net/
http://www.mpdg.org/

# 4. Proposed Minimum Information Set for Reporting Plant Biological Experimental Designs ('context metadata')

These recommendations propose a core of metadata to be submitted along with metabolomic result data.

- If certain reporting details cannot be given due to intellectual property or other commercial issues or due to due to inaccessibility of data (such as in some field trials or in studies surveying plant products for end consumers) such omissions should be stated. General descriptions should be given instead to inform the public and to enable reuse and understanding of result data in order to potentially reproduce scientific conclusions.
- If omission of metadata disables understanding and reproducing scientific conclusions, submission and reporting of metabolomic data is highly questionable and should be rejected.
- The 'Minimum Guidelines for Measuring and Reporting Environmental Parameters for Experiments on Plants in Growth Rooms and Chambers' (http:/ / ncr101.montana.edu/ min_guidelines.pdf) are acknowledged as published by the International Committee for Controlled Environment Guidelines (http:/ / ncr101.montana.edu/ )in March 2004. However, these guidelines are not regarded as mandatory but helpful for reporting plant metabolomic studies.

## 4.1. Proposed Minimum Metadata for BioSource

'the physical object that will be subjected to metabolomic analysis'

| | |
|---|---|
| Species | according to NCBI taxonomy DB ([2], [3]), http:/ / pubmedexpress.nih.gov/ Taxonomy/ taxonomyhome.html/ index.cgi. e.g. *Arabidopsis thaliana*, but not *A. thaliana*.<br><br>All necessary information on taxonomic relationships can be derived from the correct species name and thus does not need to be reported further. |
| Genotype | Subspecies information such as ecotype, cultivar, accession according to authoritative DB such as TAIR (http://www.arabidopsis.org/ ). In the case of crosses or breeding results, available pedigree information. In the case of transgenic or mutant organisms, name of the gene(s) up- or down-regulated and the GenBank Accession number(s) for the sequence of the corresponding construct(s) in addition to the parental subspecies background information.<br><br>In case of plant-pathogen interaction studies or other areas where information on multiple genomes is relevant, such metadata should be given. |
| Organ | according to the authoritative DB maintained by the Plant Ontology Consortium to be found at http:/ / www.plantontology.org/. All necessary information on organ relationships can be derived from the correct organ name and thus does not need to be reported further. |
| Organ specification | *only if* such information cannot be detailed by http:/ / www.plantontology.org/. e.g. description of a part of an organ, the |

| | |
|---|---|
| | specific location of the organ or a specific tissue of an organ. |
| Cell type | **only if: .** only if such information can be detailed in a meaningful manner, e.g. by cell type sorting or dissection. Naming according to the authoritative DB maintained by the Plant Ontology Consortium to be found at http://www.plantontology.org/ under plant_structure ontology. |
| | **only if:** such information cannot be located at this source the Cell Ontology maintained at Open Biomedical Ontologies group should be taken to be found at http://lists.sourceforge.net/lists/listinfo/obo-cell-type |
| Subcellular location | **only if:** such information can be detailed in a meaningful manner, e.g. by subcellular fractionation. Naming according to the authoritative DB (Gene Ontology Cellular Component) maintained by the Gene Ontology Consortium to be found at http:/ / www.geneontology.org/. |
| BioSource amount | mass (mg fresh weight or mg dry weight), number of cells or other measurable bulk numbers (e.g. protein content) |

# 4.2. Proposed Minimum Metadata Relative to Growth Environment

i.e. parameters that were common to all plants in a given study, but excluding those that were intentionally altered and reported under Proposed Minimum Metadata Relative to Treatment.

| | |
|---|---|
| Growth support | Soil (type, supplier), Agar (type, supplier), Vermiculite (type, supplier), hydroponic system (type, supplier, nutrients, concentrations) or other support including cell culture (media, volume, cell number per volume) |
| Growth location | Field trial (location), climate chamber (size $m^3$), greenhouse (details on accuracy of control of light, humidity and temperature conditions), other location (details on size $m^3$, accuracy of control of light, humidity and temperature conditions). |
| Growth plot design | the way to randomize the different G×E interactions |
| | either descriptive or using established nomenclature e.g. latin square. |
| Light | Light quality, source model/type, light intensity (µmol $s^{-1}m^{-2}$), luminescence (daylight) period (h) |
| | For field trials: average light parameters in growing season. Information on time and location of the field trial enables tracking of more precise information if necessary. |
| Humidity | Humidity (%) at day and at night |
| | For field trials: average humidity parameters in growing season. Information on time and location of the field trial enables tracking of more precise information if necessary. |
| Temperature | Temperature (°C) at day and at night |
| | For field trials: average temperature (°C) at day and at night in growing season. Information on time and location of the field trial enables tracking of more precise information if necessary. |
| Watering regime | Amount and time of watering per day |
| | For field trials: average rain fall in growing season. Information on time and location of the field trial enables tracking of more precise information if necessary. |
| | For hydroponic systems: frequency of solution change. |
| Nutritional regime | Amount and time of additional nutrients given to plants |
| Date(s) of plant establishment | Depending on plant study, such dates could comprise: sowing, germination, transplanting, cutting, grafting or other appropriate time stamps. |
| | Plant development stage description should accompany time |

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| | stamps, preferably using established nomenclature.[4] |
| Other specific metadata | Only if applicable and if it does not belong to Section 4.3. |
| | Examples comprise translocation of plants from one chamber to another, rotational schema of trays within a climate chamber. |
| | Examples comprise agrochemical or preventive maintenance information that are not part of Section 4.3. |

## 4.3. Proposed Minimum Metadata Relative to Treatment

| | | |
|---|---|---|
| Treatment factors | | |
| | Biotic treatment | e.g. infection (species), herbivore attack (species), competition with other plants (species) |
| | | *or other factors* |
| | Abiotic treatment | e.g. light intensity increase/decrease, cold acclimation (temperature), drought (description of residual growth support moisture, or quantitative description of reduction in watering regime), water stress, saline stress |
| | | *or other factors* |
| | Intervention treatment | e.g. application of agrochemicals, enzyme inhibitors, hormones, elicitors |
| | | *or other factors* |
| Treatment dose or intensity levels | | |
| Treatment time, time intervals and duration before harvest | | |

## 4.4. Proposed Minimum Metadata Relative to Harvest

| | |
|---|---|
| Harvest date, time | Harvest time relative to the luminescence cycle. Duration of harvest if relevant to the plant study (e.g. for volatile analysis). |
| Plant growth stage | It is advised to refer to established literature, e.g. for Arabidopsis, see [4] |
| Metabolism quenching method | Time after harvest before stopping cellular metabolism. (may be > weeks for certain post-harvest physiology experiments, may be < s for assessing high turnover metabolites). |
| | Method to stop cellular metabolism |
| Harvest method | Details of operation to gather the plant organ (sample) given in Section 4.1. |
| | Details of pooling of plant tissues for analysis |
| Sample storage | Operations to store sample (e.g. freeze-drying, grinding) prior to preparation for metabolomic analysis. |
| | Duration and temperature of storage before extraction for analysis. |

# Bibliography

[1] Nigel Hardy, Don Robertson. *Core Information for Metabolomics Reporting*. http:/ / msi-metabolomicssociety.sf.net/.

[2] Wheeler, David L. and Chappey, Colombe and Lash, Alex E. and Leipe, Detlef D. and Madden, Thomas L. and Schuler, Gregory D. and Tatusova, Tatiana A. and Rapp, Barbara A.. *Database resources of the National Center for Biotechnology Information*. *Nucl. Acids Res. %R 10.1093/nar/28.1.10*. 28. 1. 10-14. 2000.

[3] Benson, Dennis A. and Karsch-Mizrachi, Ilene and Lipman, David J. and Ostell, James and Rapp, Barbara A. and Wheeler, David L.. *GenBank*. *Nucleic Acids Research*. 28. 1. 15. 2000.

[4] Boyes, D. C. and Zayed, A. M. and Ascenzi, R. and McCaskill, A. J. and Hoffman, N. E. and Davis, K. R. and Gorlach, J.. *Growth stage-based phenotypic analysis of arabidopsis: A model for high throughput functional genomics in plants*. *Plant Cell*. 13. 7. 1499-1510. 2001.