

Metabolomics Society - Metabolomics Standards Initiative (MSI) Environmental Context Working SubGroup (ECWSG) road map

<http://msi-workgroups.sourceforge.net>

DRAFT FOR DISCUSSION

This document describes the purpose and the working strategy of the Metabolomics Society Environmental context Working SubGroup (ECWSG) in an effort to reach a broad consensus in the community on a suitable way to report environmental metabolomics experiments.

The Metabolomics Society standards initiative

The Metabolomics Society has appointed an Oversight Committee to monitor, coordinate and review the efforts of working groups (WGs) in specialist areas that will examine standardization and make recommendations. The five WGs, some of which are divided into further subgroups are listed here:

- Biological context metadata WG
- Chemical analysis WG
- Data processing WG
- Ontology WG
- Data exchange WG

The structure of the WGs thus follows the general "workflow" model in metabolomics: from a description of the study design to sample workup, data acquisition, processing and export, bound together by controlled vocabularies and relationships between the terms used.

ECWSG statement of purpose

The Environmental Context Working SubGroup (ECWSG) is a subgroup of the Biological Context Metadata Working Group. The ECWSG seeks to facilitate the consistent annotation of environmental metabolomics experiments in collaboration with the other context groups (Plant, Mammalian, Microbe) and the rest of the MSI community. This Working Group considers Environmental Metabolomics as the application of metabolomics to the fields of environmental biology and toxicology.

Operating plan

The ECWSG will tackle this issue by:

1. Evaluating the MIAME/Env specification for adoption by the ECWSG
2. Determining if and how the Env specification needs to be altered / extended for the sake of describing metabolomic (as opposed to transcriptomic) experiments

The developmental process will require the following groups of people to provide input:

- The ECWSG members as developers of the Env extension of the Core Information for Metabolomics Reporting (CIMR)
- Standardization experts/knowledge engineers to provide advice about the engineering of the specification and identify potential overlap with other 'omic specifications (e.g. MIAME, HUPI-PSI, MIGS)
- Environmental metabolomics practitioners to provide use cases, validate the selected descriptors, and eventually produce compliant annotations

Operating principles

The ECWSG will seek to represent the views of community members working in the area of environmental biology using metabolomics approaches in an unbiased and open fashion. The group will integrate and harmonize with other WGs within the standardization initiative. Communications will be frequent, respectful but candid and widely distributed. Every effort will be made to meet group goals in a timely fashion, although no central fund exists for this initiative and the members participate on a volunteer basis.

To achieve these goals the ECWSG will:

- Work co-operatively, maintain a mailing list and a website with the names of participating members to remain approachable, inclusive and transparent while the size of the group and the complexity of the tasks increase.
- Produce and maintain a set of documents - which are either common practice descriptions, or recommendations - to ensure that the statements from this group are clear, accurate and accessible to the community in a timely fashion.

- Leverage on previous and relevant work in other omics studies, and recent metabolomics standardization efforts.
- Represent the metabolomics domain within a larger, international effort developing integrated standards for 'omics data within the MICheck project (micheck.sf.net) and beyond

Strategic plan

Phase 1 – Initial evaluation of the Env specification

The first two phases focus on the evaluation of the existing Env specification, the identification of suitable case studies in environmental metabolomics, and the application of Env to these case studies.

The MIAME/Env specification (http://envgen.nox.ac.uk/miame/miame_env.html) has been developed to extend the MIAME specification for the sake of describing environmental transcriptomic experiments. While originally applied to transcriptomics, the Env specification is essentially technology independent and could be applied to the description of any relevant data type. It is currently being incorporated into the Genomic Standards Consortium (GSC) "Minimal Information about a Genome Sequence" (MIGS) specification (gensc.sf.net). The Members of the ECWSG will examine Env and consider its relevance to environmental metabolomics experiments.

Field Code Changed

Phase 2 – Use case development

Two or three use cases will be selected from members of the ECWSG and the wider community. Use cases will be described and posted to the ECWSG website. In a second step, we will attempt to apply Env to each case study, and a report will also be written and posted. Any requirements for adapting / extending Env will be highlighted.

Phase 3 – Evaluation of Env in the context of the other MSI Biological context WG's

We will evaluate Env in the context of the other biological context WG's to identify any overlaps / gaps in our reporting.

Phase 4 – Adaptation / Extension of the Env specification

The ECWSG's ultimate goal is to identify the core set of descriptors necessary to correctly and adequately describe an environmental metabolomics experiment. To do so, after evaluating Env through group discussions, via its application to case studies, and by discussion with the other Biological context WG's, we will adapt or extend it in anyway necessary.

The larger scientific community will best be served if the resulting specification overcomes duplications across omics domains where commonality of the concepts exists. To achieve this goal the ECWSG will interact with the MICheck (micheck.sf.net) project as well as with individual groups (i.e. MGED, HUPO-PSI, GSC).

MSI ECWSG members

Dawn Field (NERC Environmental Bioinformatics Centre, UK), MSI ECWSG Chair (temporary)

Norman Morrison (NERC Environmental Bioinformatics Centre, UK) MSI ECWSG Chair (after Oct 2006)

Mark Viant (University of Birmingham, UK) MSI ECWSG Co-Chair

Daniel Schober (EBI, UK)

Susanna-Assunta Sansone (EBI, UK and MGED Society), MSI OWG Chair

Denis Rubtsov (University of Cambridge, UK)

David Hancock (NERC Environmental Bioinformatics Centre, UK)

Matthew Davey (University of Sheffield, UK)

Tim Collette (U.S. Environmental Protection Agency, National Exposure Research Laboratory, US)

Dan Bearden (National Ocean Service, Center for Coastal Environmental Health and Biomolecular Research, US)

The ECWSG's expertise covers the following areas:

- Environmental metabolomics, computational biology, systems biology
- Knowledge representation and ontology
- Modeling, software development, data analysis