

# MIBBI, MIASE and all that

Nicolas Le Novère, EMBL-EBI

"Perfection is achieved, not when there is nothing more to add, but when there is nothing left to take away."

Antoine De Saint Exupery



- List of the core set of information that has to be provided with a data-set, so that a user is able to make sensible use of it.
- "Minimal": Only the information shared by all the providers/users of this type of data should be considered.

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 "Standard": The information should be provided in a form that can be fully interpreted by all.





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#### \_computational BIOLOGY

# COMMENTARY

# Promoting coherent minimum reporting guidelines for biological and biomedical investigations: the MIBBI project

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The Minimum Information for Biological and Biomedical Investigations (MIBBI) project provides a resource for those exploring the range of extant minimum information checklists and fosters coordinated development of such checklists.

o fully understand the context, methods, data and conclusions that pertain to an experiment, one must have access to a range of background information. However, the current diversity of experimental designs and analytical techniques complicates the discovery and evaluation of experimental data; furthermore, the increasing rate of production of those data compounds the problem. Community opinion increasingly favors that a regularized set of the available metadata ('data about the data') per-

guidelines for reporting proteomics experiments and describing systems biology models are gaining broader support in their respective database communities<sup>8,9</sup>; and progress is being made toward the standardization of the reporting of clinical trials in the medical literature<sup>10</sup>. Such minimum information checklists promote transparency in experimental reporting, enhance accessibility to data and support effective quality assessment, increasing the general value of a body of work (and the comoverlaps in scope and arbitrary decisions on wording and substructuring inhibit their use in combination. These issues present difficulties for checklist users, especially those who routinely combine information from several disciplines. Here we explore some of the issues arising from the development of checklists in relative isolation, discuss the potential benefits of greater coordination and describe the mechanisms we have put in place to facilitate such coordination. In summary, we present



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#### search

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#### The MIBBI Foundry

Towards the next generation of MI quidelines for the biosciences

#### **Related** resources

MIBBI search

A Google™ Custom

Links to other cross-domain projects, policy statements and sundry useful material



How to post to the MIBBI discussion forum, or join the Foundry developers' mailing list

# http://www.mibbi.org



## Project News

discussion

article

BMC journals recommend MIBBI in their 'Instructions to Authors' (example @)

history

Free download: The MIBBI paper (Nature Biotechnology)

### Site navigation

#### The MIBBI Portal

Access to Minimum Information guidelines for diverse bioscience domains

view source

About us A contextualisation of the project, our rules and regulations, and our publications and talks.



# **Project news**

Announcements relating to the project, such as new registrations, meetings, etc.

## Discussion



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What links here				
<ul> <li>What links here</li> <li>Related changes</li> <li>Upload file</li> <li>Special pages</li> <li>Printable version</li> <li>Permanent link</li> </ul>	MIAME	Minimum Information About a Microarray Experiment		
	MIAME/Env	MIAME / Environmental transcriptomic experiment		
	MIAME/Nutr	MIAME / Nutrigenomics		
	MIAME/Plant	MIAME / Plant transcriptomics		
	MIAME/Tox	MIAME / Toxicogenomics		
	MIAPA	Minimum Information About a Phylogenetic Analysis		
	MIAPAR	Minimum Information About a Protein Affinity Reagent		
	MIAPE	Minimum Information About a Proteomics Experiment		
	MIARE	Minimum Information About a RNAi Experiment		
	MIASE	Minimum Information About a Simulation Experiment		
	MIENS	Minimum Information about an ENvironmental Sequence		
	MIFlowCyt	Minimum Information for a Flow Cytometry Experiment		
	MIGen	Minimum Information about a Genotyping Experiment		
	MIGS	Minimum Information about a Genome Sequence	=	
	MIMIx	Minimum Information about a Molecular Interaction Experiment		
	МІМРР	Minimal Information for Mouse Phenotyping Procedures		
	MINI	Minimum Information about a Neuroscience Investigation		
	MINIMESS	Minimal Metagenome Sequence Analysis Standard		
	MINSEQE	Minimum Information about a high-throughput SeQuencing Experiment		
	MIPFE	Minimal Information for Protein Functional Evaluation		
	MIQAS	Minimal Information for QTLs and Association Studies		
	MIqPCR	Minimum Information about a quantitative Polymerase Chain Reaction experiment		
	MIRIAM	Minimal Information Required In the Annotation of biochemical Models		
		Minimum Information Specification For In Situ Hybridization and		

# MIRIAM





- Specifically about encoding & annotation
- Limited to models that can be simulated
- Effort arose from a meeting organized by Andrew Finney during ICSB 2004
- Not specific to SBML; applicable to any structured model format



## PERSPECTIVE

#### Minimum information requested in the annotation of biochemical models (MIRIAM)

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Most of the published quantitative models in biology are lost for the community because they are either not made available or they are insufficiently characterized to allow them to be reused. The lack of a standard description format. lack of stringent reviewing and authors' carelessness are the main causes for incomplete model descriptions. With today's increased interest in detailed biochemical models. it is necessary to define a minimum quality standard for the encoding of those models. We propose a set of rules for curating quantitative models of biological systems. These rules define procedures for encoding and annotating models represented in machine-readable form. We believe their application will enable users to (i) have confidence that curated models are an accurate reflection of their associated reference descriptions, (ii) search collections of curated models with precision, (iii) quickly identify the biological phenomena that a given curated model or model constituent represents and (iv) facilitate model reuse and composition into large subcellular models.

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New York, New York 10021, USA. <sup>6</sup>Center for Genomic Sciences, Universidad Nacional Autónoma de México, Av. Universidad s/n, Cuernavaca, Morelos, During the genomic era we have witnessed a vasi increase in availability of large amounts of quantitative data. This is motivating a shift in the focus of molecular and cellular research from qualitative descriptions of biochemical interactions towards the quantification of such interactions and their dynamics. One of the tenets of systems biology is the use of quantitative models (see Box 1 for definitions) as a mechanism for capturing precise hypotheses and making predictions<sup>1,2</sup>. Many specialized models exist that attempt to explain aspects of the cellular machinery. However, as has hypened with other types of biological information, such as sequences, macromolecular structures or

#### Box 1 Glossary

Some terms are used in a very specific way throughout the article. We provide here a precise definition of each one.

Quantitative blochemical model. A formal model of a biological system, based on the mathematical description of its molecular and cellular components, and the interactions between those components.

Encoded model. A mathematical model written in a formal machine-readable language, such that it can be systematically parsed and employed by simulation and analysis software without further human translation.

MIRIAM-compliant model. A model that passes all the tests and fulfills all the conditions listed in MIRIAM.

Reference description. A unique document that describes, or references the description of the model, the structure of the model, the numerical values necessary to instantiate a simulation from the model, or to perform a mathematical analysis of the model, and the results one expects from such a simulation or analysis.

Curation process. The process by which the compliance of an encoded model with MIRIAM is achieved and/or verified. The curation process may encompass some or all of the following tasks: encoding of the model, verification of the reference correspondence and annotation of the model.

Reference correspondence. The fact that the structure of a model and the results of a simulation or an analysis match the information present in the reference description.

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- <u>Research applications</u>: Yeast Metabolic Model (Herrgård M.J. et al (2008), *Nat Biotechnol* 26: 1155-1160), : 2152 species, 1857 reactions, 4861
   MIRIAM annotations. Human Metabolic Model: 4889 species, 8866 reactions, **66968** MIRIAM annotations
- <u>Data resources using MIRIAM</u>: BioModels Database (kinetic models), PSI consortium (protein interactions), Reactome (pathways), SABIO-RK (reaction kinetics)
- <u>Software using MIRIAM</u>: COPASI (Simulation), Snazzer (Network analysis, Simulations), Systems Biology Workbench (model design and simulation), The Virtual Cell (Simulation), SBMLsemantics, libSBMLannotation, SAINT
- <u>Statistics of usage of MIRIAM Resources</u>: Web Interface: 13 494 page requests in 2008, 245.15 MB data transferred, 1 539 unique users. WebServices: 578 620 requests



# EMBL-EBI Mosaic of standards for computational modeling





- List and structure of biological entities and processes
- Mathematical descriptions of the amounts and transformations

# Missing:

- What to do with the models
- How to do it
- What to do with the results







## Edelstein et al 1996 (BIOMD00000002)







Edelstein et al 1996 (BIOMD00000002)



Huang & Ferrell (BIOMD00000009)







## Edelstein et al 1996 (BIOMD000000002)



## Huang & Ferrell (BIOMD00000009)



## Ueda, Hagiwara, Kitanol 2001 (BIOMD000000022)







## Edelstein et al 1996 (BIOMD000000002)



Huang & Ferrell (BIOMD00000009)



## Ueda, Hagiwara, Kitanol 2001 (BIOMD000000022)



# Bornheimer et al 2004 (BIOMD000000086)





MIASE aims at describing the information needed to run and repeat a numerical simulation experiment derived from a given quantitative model.

What information do-we need to achieve that goal?

- Information about the models to use
- Information about the simulation task to perform
- Information about result processing

More information at:

http://www.ebi.ac.uk/compneur-srv/miase

