MetaboLights: Quick tour

Kenneth Haug [1]

- Systems
- Chemical biology
- Beginner
- 0.5 hour

This quick tour provides a brief introduction to the EBI's metabolomics resource: MetaboLights [2].

Learning objectives:

- A basic understanding of MetaboLights and how to use it

What is MetaboLights?

MetaboLights [3] is the first general purpose, open access [4] repository for metabolomics [5] studies, their raw experimental data and associated metadata [6], maintained by one of the major open access data providers in molecular biology (Figure 1).

The identification and quantification of metabolites can provide unique insights into the metabolic processes that are taking place in the cellular environment. Metabolic profiles [7] taken from body fluids have the potential to act as biomarkers for many different diseases, an approach that has already shown value in, for example, heart disease and diabetes, the effects of diet and interactions with the environment.

MetaboLights consists of two distinct layers:

1) a repository, enabling the metabolomics community to share findings, data and protocols for any form of metabolomics study;

2) a reference layer of curated knowledge about metabolite structures and their reference spectra, as well as their biological roles, locations, concentrations, and raw data [8] from metabolic experiments.

The effectiveness of metabolomic profiling methods depends on the availability of public open data across a broad range of experimental methods and conditions. The MetaboLights repository seeks to fulfil this requirement.

MetaboLights is specifically designed to build on prior art and to extensively collaborate with the existing databases, ensuring that data are exchanged and that assimilation efforts target gaps in the knowledge available worldwide.
What can I do with MetaboLights?

With MetaboLights you can:

- Find metabolites and related metablomics studies by searching a wide range of associated metadata [6].
- Filter your search results on species, techniques and metabolites.
- Submit public or private studies.
- Receive a stable and unique accession [9] number that can be used as a publication reference.
- Share private studies with collaborators/peer reviewers.
- Retrieve molecular information from ChEBI [10] or other linked compound databases.

Searching and visualising data in MetaboLights

Search results

From the MetaboLights homepage [2] you can search for an extensive set of associated information for the studies stored in MetaboLights (Figure 2). This includes information about submitters and authors, publication references, the study design, protocols applied, names of data files included, platform information and metabolite information. The metabolite information includes a description,
external database identifiers, formula and intensity or concentration, and where the metabolite was identified in the sample.

**Figure 2** A sub-section of the search results page in MetaboLights, highlighting some of the search filters available.

**Browse the repository**
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Figure 3: Search results: browsing all public studies in MetaboLights.

Study details page
Figure 4  Samples submitted in an NMR study about human type 2 diabetes.

Study details page: protocols
Getting data from MetaboLights

All public studies and associated data in MetaboLights are freely available for download. You can further modify these data as you wish.

There are two main methods for downloading studies:

- directly download a zipped archive from the study details page;
- download individual files and folders from our FTP site [11].

Submitted data is encoded in the standardised and open ISA-Tab format [12].

Submitting data to MetaboLights

MetaboLights accepts submissions in ISA-tab format.

For more information, please see our comprehensive submissions guide [13].

In general, to submit data you will have to create an account, download the submissions tool and start creating your study.

The required steps can be found in the submisisons guides - below are the links to specific documents:
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- **Overview** [14]
- **Download and set up ISACreator** [15]
- **Setup and create NMR study** [16]
- **Setup and create GC/MS study** [17]
- **Setup and create LC/MS study** [18]
- **Submit your study to MetaboLights** [19]
- **Curation status and automatic validations** [20]
- **Frequently asked questions (FAQ)** [21]
  - 问答 [22]

**Your feedback**

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**Get help and support on MetaboLights**

**Support**

- For comments, suggestions or help requests, please use our [feedback form] [23].
- For source code, feature requests and bug reports, see the MetaboLights [SourceForge pages] [24].

**Collaborators**

MetaboLights submissions use the [ISA software suite] [25] so experimental data gets submitted in [ISA-Tab] [25] format.

The MetaboLights project is a member of [isacommons] [26], the ISA community.

![The Investigation/Study/Assay (ISA) infrastructure is the first general purpose format and freely available desktop software suite that assists in the reporting and local management of experimental metadata from studies using one or more technologies. Metadata types that can be captured by ISA-tab include sample characteristics, the technology and measurement types used, and sample-to-data relationships. ISA-Tab is built for experimentalists, curators and software developers.](image)

**References**

Funding

The development of MetaboLights is funded by the BBSRC [31], grant reference BB/L024152/1 [32]. Previous BBSRC grant reference is BB/I000933/1 [33]. The funding is for a project that will instantiate, at the European Bioinformatics Institute (EBI) in Hinxton, Cambridge, UK, the MetaboLights metabolomics database with various components focused on both data standards and primary experimental data. MetaboLights is cross-species, cross-application and will cover all relevant analytical methods.

MetaboLights is a joint development between the Claire O'Donovan group [34] at the European Bioinformatics Institute and the Griffin group [35] in Cambridge.

Contributors

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Ken Haug joined the EBI in 2009 and is currently a Project Manager and Software Engineer in the Cheminformatics and Metabolism group. Ken studied IT in Oslo before joining Oracle in Norway as an IT Manager and later a Solution Architect for Oracle Consulting. 10 years ago Ken moved to the UK and worked for the next 6 years for an Oracle-focused consultancy in London/Reading, working on various projects as a customer-facing Project Manager and Consultant.

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Links
[1] http://www.ebi.ac.uk/training/online/trainers/kenneth
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[9] http://www.ebi.ac.uk/training/online/glossary/accession
[10] http://www.ebi.ac.uk/training/online/glossary/chebi