

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).

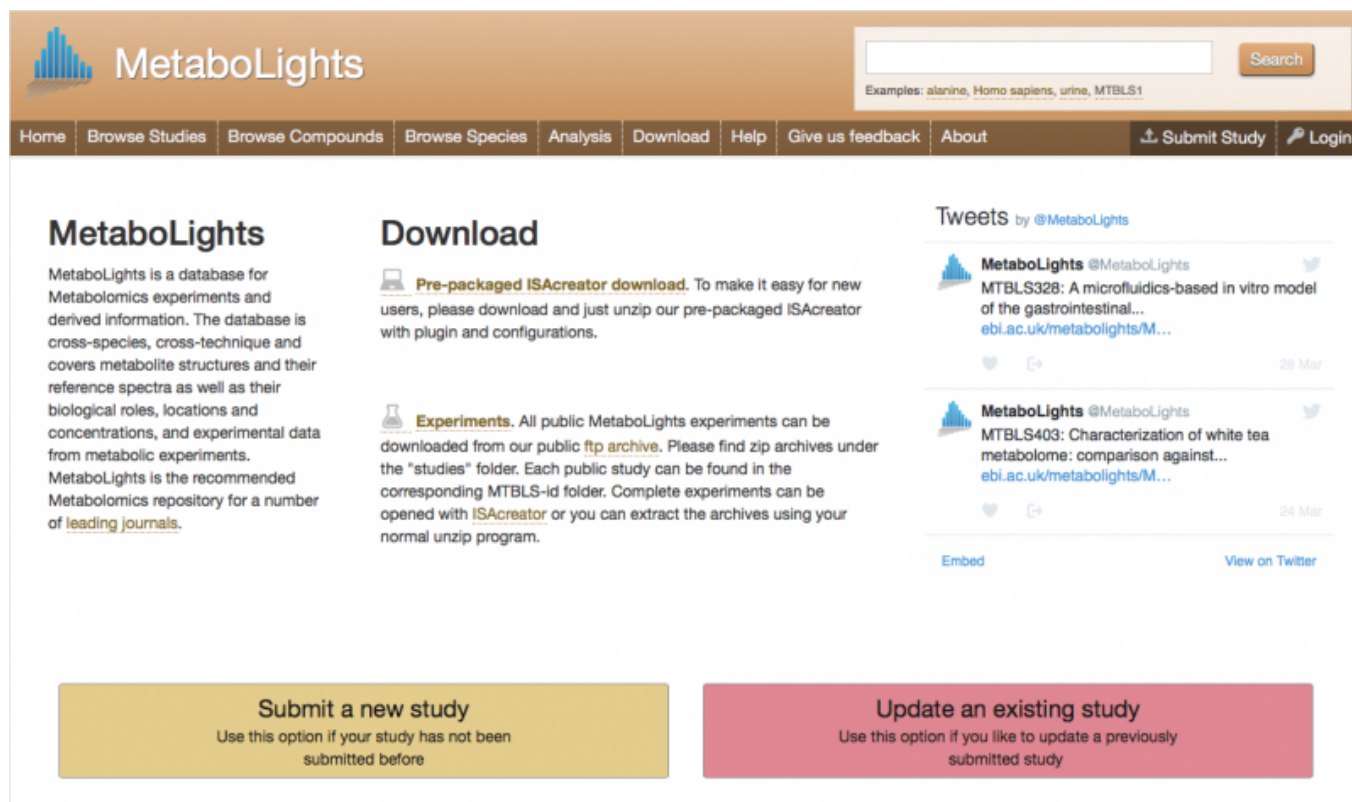
The identification and quantification of metabolites can provide unique insights into the metabolic processes that are taking place in the cellular environment. Metabolic [profiles](#) [7] taken from body fluids have the potential to act as biomarkers for many different diseases, an approach that has 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.



MetaboLights

MetaboLights is a database for Metabolomics experiments and derived information. The database is cross-species, cross-technique and covers metabolite structures and their reference spectra as well as their biological roles, locations and concentrations, and experimental data from metabolic experiments. MetaboLights is the recommended Metabolomics repository for a number of [leading journals](#).

Download

Pre-packaged ISAcceptor download. To make it easy for new users, please download and just unzip our pre-packaged ISAcceptor with plugin and configurations.

Experiments. All public MetaboLights experiments can be downloaded from our public [ftp archive](#). Please find zip archives under the "studies" folder. Each public study can be found in the corresponding MTBLS-id folder. Complete experiments can be opened with [ISAcceptor](#) or you can extract the archives using your normal unzip program.

Tweets by @MetaboLights

MetaboLights @MetaboLights
MTBLS328: A microfluidics-based in vitro model of the gastrointestinal...
ebi.ac.uk/metabolights/M...
28 Mar

MetaboLights @MetaboLights
MTBLS403: Characterization of white tea metabolome: comparison against...
ebi.ac.uk/metabolights/M...
24 Mar

Submit a new study
Use this option if your study has not been submitted before

Update an existing study
Use this option if you like to update a previously submitted study

Figure 1 [MetaboLights homepage](#) [2].

What can I do with MetaboLights?

With MetaboLights you can:

- Find metabolites and related metabolomics 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.
- Download public [metabolomics](#) [5] studies for further analysis.
- 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.

The screenshot displays the MetaboLights search results page. At the top, the MetaboLights logo is visible on the left, and a search bar on the right contains the text 'Homo sapiens' with a 'Search' button. Below the search bar, a navigation menu includes links for Home, Browse Studies, Browse Compounds, Browse Species, Analysis, Download, Help, Give us feedback, and About. On the right side of the menu are links for 'Submit Study' and 'Login'.

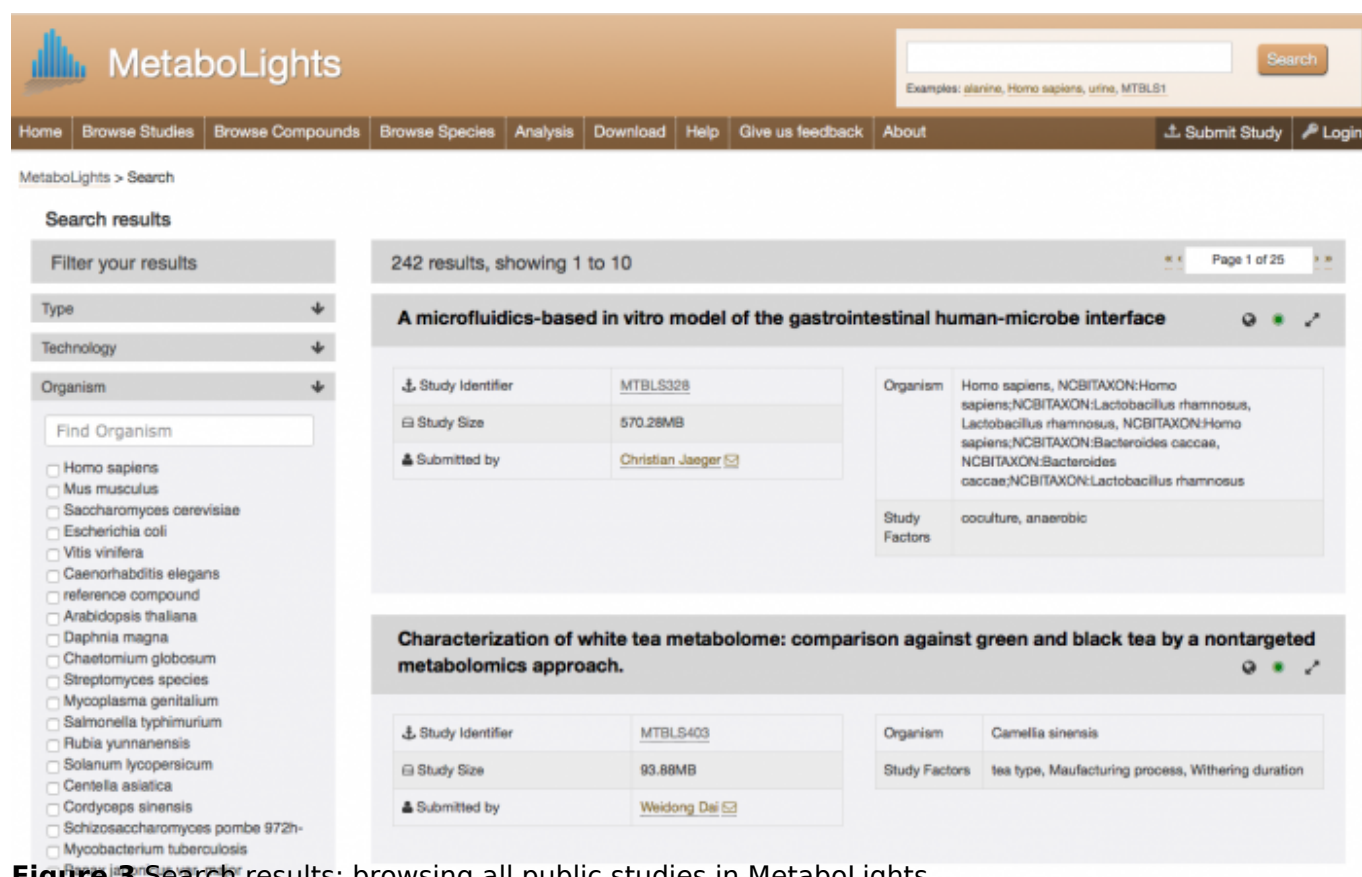
The main content area shows 'MetaboLights > Search' and 'Search results'. A 'Filter your results' sidebar on the left includes dropdown menus for 'Type', 'Technology', 'Organism', 'Organism Part', 'Validations Status', and 'Validations Status Details'. The 'Technology' dropdown is expanded, showing options for 'mass spectrometry' and 'NMR spectroscopy'. The main results area displays '3235 results, showing 1 to 10' and 'Page 1 of 324'. A button 'Show more data from EMBL-EBI' is located at the top right of the results area.

Two results are highlighted:

- Hyaluronic Acid**: The chemical structure is shown on the left. To the right, the 'COMPOUND ACCESSION' is 'MTBLC16336', and it is 'Identified in CHEBI:16336'.
- Lysophosphatidylcholine 18:2**: The chemical structure is shown on the left. To the right, the 'COMPOUND ACCESSION' is 'MTBLC64549', and it is 'Identified in MTBLS4, CHEBI:64549'. A 'DESCRIPTION' section states: 'A lysophosphatidylcholine in which the acyl group (position not specified) contains 18 carbons and 2 double bonds.'

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

Browse the repository



The screenshot shows the MetaboLights website interface. At the top, there is a navigation bar with links: Home, Browse Studies, Browse Compounds, Browse Species, Analysis, Download, Help, Give us feedback, About, Submit Study, and Login. A search bar is located on the right with the text "Examples: alanine, Homo sapiens, urine, MTBLS1".

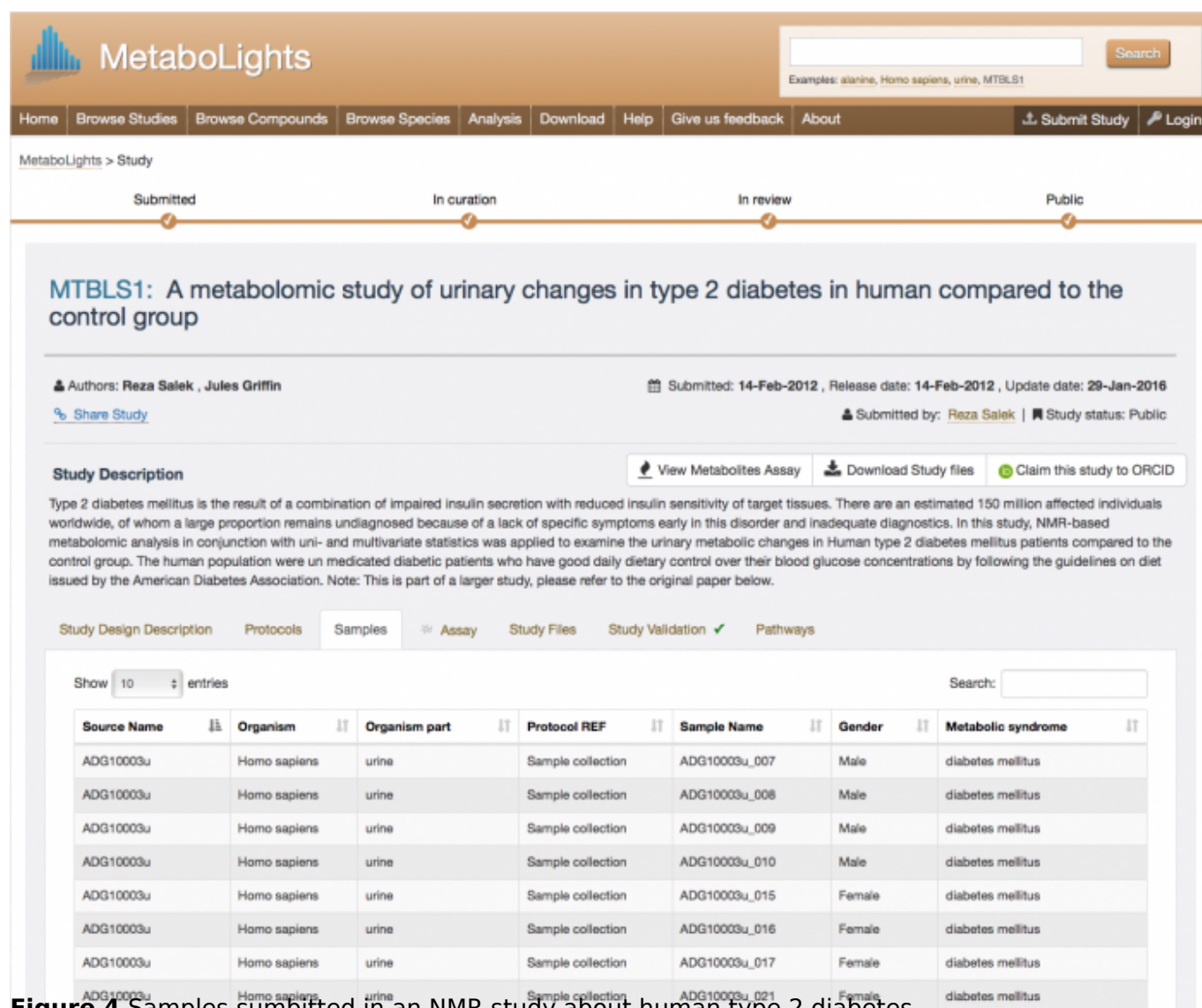
Below the navigation bar, the page title is "MetaboLights > Search". The main content area is titled "Search results" and shows "242 results, showing 1 to 10". On the left, there is a sidebar with filters: Type, Technology, and Organism. The Organism filter is expanded, showing a list of organisms with checkboxes: Homo sapiens, Mus musculus, Saccharomyces cerevisiae, Escherichia coli, Vitis vinifera, Caenorhabditis elegans, reference compound, Arabidopsis thaliana, Daphnia magna, Chaetomium globosum, Streptomyces species, Mycoplasma genitalium, Salmonella typhimurium, Rubia yunnanensis, Solanum lycopersicum, Centella asiatica, Cordyceps sinensis, Schizosaccharomyces pombe 972h-, and Mycobacterium tuberculosis.

The main results area displays two study cards. The first card is titled "A microfluidics-based in vitro model of the gastrointestinal human-microbe interface". It shows the Study Identifier as MTBLS328, Study Size as 570.28MB, and Submitted by as Christian Jaeger. The Organism field lists: Homo sapiens, NCBITAXON:Homo sapiens;NCBITAXON:Lactobacillus rhamnosus, Lactobacillus rhamnosus, NCBITAXON:Homo sapiens;NCBITAXON:Bacteroides caccae, NCBITAXON:Bacteroides caccae;NCBITAXON:Lactobacillus rhamnosus. The Study Factors field lists: coculture, anaerobic.

The second card is titled "Characterization of white tea metabolome: comparison against green and black tea by a nontargeted metabolomics approach." It shows the Study Identifier as MTBLS403, Study Size as 93.88MB, and Submitted by as Weidong Dai. The Organism field lists: Camellia sinensis. The Study Factors field lists: tea type, Manufacturing process, Withering duration.

Figure 3 Search results: browsing all public studies in MetaboLights.

Study details page



MetaboLights

Examples: alanine, Homo sapiens, urine, MTBLS1

Home Browse Studies Browse Compounds Browse Species Analysis Download Help Give us feedback About Submit Study Login

MetaboLights > Study

Submitted In curation In review Public

MTBLS1: A metabolomic study of urinary changes in type 2 diabetes in human compared to the control group

Authors: Reza Salek, Jules Griffin Submitted: 14-Feb-2012, Release date: 14-Feb-2012, Update date: 29-Jan-2016

Share Study Submitted by: Reza Salek Study status: Public

Study Description View Metabolites Assay Download Study files Claim this study to ORCID

Type 2 diabetes mellitus is the result of a combination of impaired insulin secretion with reduced insulin sensitivity of target tissues. There are an estimated 150 million affected individuals worldwide, of whom a large proportion remains undiagnosed because of a lack of specific symptoms early in this disorder and inadequate diagnostics. In this study, NMR-based metabolomic analysis in conjunction with uni- and multivariate statistics was applied to examine the urinary metabolic changes in Human type 2 diabetes mellitus patients compared to the control group. The human population were un medicated diabetic patients who have good daily dietary control over their blood glucose concentrations by following the guidelines on diet issued by the American Diabetes Association. Note: This is part of a larger study, please refer to the original paper below.

Study Design Description Protocols **Samples** Assay Study Files Study Validation Pathways

Show 10 entries Search:

Source Name	Organism	Organism part	Protocol REF	Sample Name	Gender	Metabolic syndrome
ADG10003u	Homo sapiens	urine	Sample collection	ADG10003u_007	Male	diabetes mellitus
ADG10003u	Homo sapiens	urine	Sample collection	ADG10003u_008	Male	diabetes mellitus
ADG10003u	Homo sapiens	urine	Sample collection	ADG10003u_009	Male	diabetes mellitus
ADG10003u	Homo sapiens	urine	Sample collection	ADG10003u_010	Male	diabetes mellitus
ADG10003u	Homo sapiens	urine	Sample collection	ADG10003u_015	Female	diabetes mellitus
ADG10003u	Homo sapiens	urine	Sample collection	ADG10003u_016	Female	diabetes mellitus
ADG10003u	Homo sapiens	urine	Sample collection	ADG10003u_017	Female	diabetes mellitus
ADG10003u	Homo sapiens	urine	Sample collection	ADG10003u_021	Female	diabetes mellitus

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

Study details page: protocols

Study Design Description	Protocols	Samples	Assay	Study Files	Study Validation	Pathways
Show 10 entries Search: <input type="text"/>						
Protocol	Description					
Extraction	For the human studies, midstream urine (~15 ml) samples were collected and frozen from each volunteer. In total, 84 samples were collected from 12 healthy volunteers (7 time points, 6 males and 4 females) and 50 samples from 30 T2DM patients (1–3 time points, 17 males and 13 females) with well-controlled blood glucose maintained at normal concentrations by diet, following the guidelines issued by the American Diabetes Association, rather than medication. The healthy subjects were aged 18–55 yr, had a body mass index (BMI) ≥19 and ≤30 kg/m ² and a body mass ≥50 kg and ≤113 kg, and were free from any major disease or pregnancy. The T2DM patients were aged 30–65 yr (mean 56 ± 9 yr), had a BMI >25 and <40 kg/m ² , weighed between 65 and 140 kg (mean 95 ± 19 kg), and were taking at most one oral anti-diabetic drug. T2DM patients agreed to stop treatment with oral anti-diabetic agents during the study. Subjects went through a washout period of 4 wk before sample collection and abstained from alcohol during the study; diet was controlled throughout the study.					
NMR sample	Aliquots of 400 µl urine samples were made up to 600 µl with phosphate buffer (0.2 M, pH 7.4) and any precipitate removed by centrifugation. In total, 500 µl of supernatant were transferred to 5-mm NMR tubes with 100 µl of sodium 3-trimethylsilyl-(2,2,3,3-tetrahydroxy-1-propionate) (TSP)/D ₂ O/sodium azide solution (0.05% wt/vol TSP in D ₂ O and 1% wt/vol sodium azide).					
NMR spectroscopy	The spectra of human urine samples were acquired on a Bruker DRX700 NMR spectrometer using a 5 mm TXI ATMA probe at a proton frequency of 700.1 MHz and ambient temperature of 27 °C.					
NMR assay	A 1D NOESY presaturation pulse sequence was used to analyze the urine samples. For each sample 128 transients were collected into 64k data points using a spectral width of 14,005 kHz (20 ppm) and an acquisition time of 2.34 s per FID.					
Data transformation	Spectra were processed using ACD/1D NMR Manager 8.0 with Intelligent Bucketing Integration (Advanced Chemistry Development, Toronto, ON, Canada). Spectra were integrated 0.20–9.30 ppm excluding water (4.24–5.04 ppm), glucose (3.19–3.99 ppm, 5.21–5.27 ppm), and urea (5.04–6.00 ppm). Intelligent bucketing ensures that bucket edges do not coincide with peak maxima, preventing resonances from being split across separate integral regions; a 0.04 ppm bucket width and a 50% looseness factor were used. All spectra were normalized to total area excluding the water, urea, and glucose regions.					
Metabolite identification	Assignments were confirmed by two dimensional spectroscopy including homonuclear 1H-1H Correlation Spectroscopy (COSY), 1H-13C Heteronuclear Signal Quantum Coherence (HSQC) and 1H-13C Heteronuclear Multiple Bond Correlation (HMBC) Spectroscopy.					
Sample collection	For the human studies, midstream urine (~15 ml) samples were collected and frozen from each volunteer. In total, 84 samples were collected from 12 healthy volunteers (7 time points, 6 males and 4 females) and 50 samples from 30 T2DM patients (1–3 time points, 17 males and 13 females) with well-controlled blood glucose maintained at normal concentrations by diet, following the guidelines issued by the American Diabetes Association, rather than medication. T2DM patients agreed to stop treatment with oral anti-diabetic agents during the study. Subjects went through a washout period of 4 wk before sample collection and abstained from alcohol during the study; diet was controlled throughout the study.					

Showing 1 to 7 of 7 entries

Figure 5 MetaboLights also contains information about the protocols applied to a study.

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 submissions guides - below are the links to specific documents:

- [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]
 - [□□□□□□](#) [22]

Your feedback

Please tell us what you thought about this course. Your feedback is invaluable and helps us to improve our courses and thus enhance your learning experience.

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 [isacommuns](#) [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.

References

- Haug, K. et al. (2013). [MetaboLights—an open-access general-purpose repository for metabolomics studies and associated meta-data](#). [27] Nucleic Acids Res. 41 (D1) D781-6.
- Salek RM, et al. (2013). [The MetaboLights repository: curation challenges in metabolomics](#). [28] Database (Oxford), bat029.
- Steinbeck, C. et al. (2012). [MetaboLights: towards a new COSMOS of metabolomics data management](#). [29] Metabolomics (8), 757-760.
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121-126.

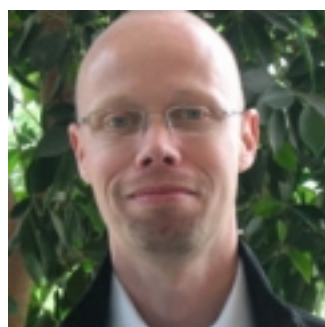
Funding

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



[1]

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EMBL-EBI

MetaboLights Project Manager and Software Engineer

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.

Source URL: <https://www.ebi.ac.uk/training/online/course/metabolights-quick-tour-0>

Links

- [1] <https://www.ebi.ac.uk/training/online/trainers/kenneth>
- [2] <http://www.ebi.ac.uk/metabolights/>
- [3] <http://www.ebi.ac.uk/metabolights>
- [4] <https://www.ebi.ac.uk/training/online/glossary/open-access>
- [5] <https://www.ebi.ac.uk/training/online/glossary/metabolomics>
- [6] <https://www.ebi.ac.uk/training/online/glossary/metadata>
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- [8] <https://www.ebi.ac.uk/training/online/glossary/raw-data>
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- [10] <https://www.ebi.ac.uk/training/online/glossary/chebi>
- [11] <ftp://ftp.ebi.ac.uk/pub/databases/metabolights/studies/>
- [12] <http://isatab.sourceforge.net/format.html>
- [13] <http://www.ebi.ac.uk/metabolights/help>

- [14] https://docs.google.com/document/d/1gNITtVK_lkwa14HDfPG04OfqbMo7NbnuulR4yjaZePo/edit?usp=sharing
- [15] <https://docs.google.com/document/d/1iXfj3VmXXvubxpSnSlj5vzJpsXE1ZNxOwcwovFYwPxs/edit?usp=sharing>
- [16] https://docs.google.com/document/d/17DjTZRv-MAuRFDqkLPu3_3xC7dExA7Vli0QEtBNpbGY/edit?usp=sharing
- [17] <https://docs.google.com/document/d/1s7X5tLF0q0tXm76LMbBovW1NReOdmWoOGLO3bm7xm6E/edit?usp=sharing>
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- [19] <https://docs.google.com/document/d/1Gnv0pvYpbYOY1pv-XZKXanCYMNIIMhPgVUEHCJ4gm98/edit?usp=sharing>
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- [22] <ftp://ftp.ebi.ac.uk/pub/databases/metabolights/documentation/MetaboLights%2020170224.pdf>
- [23] <http://www.ebi.ac.uk/metabolights/contact>
- [24] <https://sourceforge.net/projects/metabolomes/>
- [25] <http://www.isa-tools.org/>
- [26] <http://www.isacommons.org/>
- [27] <http://europepmc.org/abstract/MED/23109552>
- [28] <http://europepmc.org/abstract/MED/23630246>
- [29] <http://europepmc.org/abstract/MED/23060735>
- [30] <http://europepmc.org/abstract/MED/22281772>
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- [34] <https://www.ebi.ac.uk/about/people/claire-odonovan>
- [35] <http://www.metabolomics.bioc.cam.ac.uk/metabolomics/>