An introduction to MetaboLights

EMBL-EBI Metabolomics Team

www.ebi.ac.uk

EMBL-EBI

Metabolomics Resources

hmdb
The Human Metabolome Database

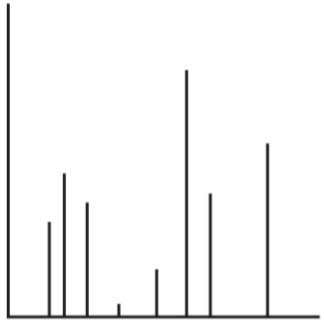
LIPID MAPS

METLIN

KEGG Kyoto Encyclopedia of Genes and Genomes

GNPS

Spectral Libraries



Analysis Tools

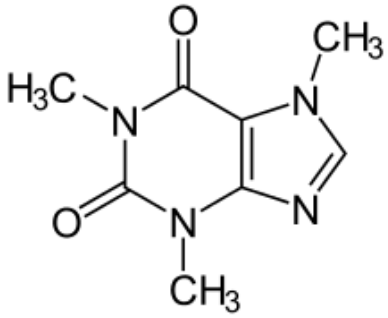
MetaboLights

PhenoMeNal
Large-Scale Computing for Medical Metabolomics

4 Wm
Workflow4metabolomics

MetaboAnalyst 4.0
Statistics
Visualization
Integration
Biomarker
Pathway
Function

Metabolite Knowledgebases

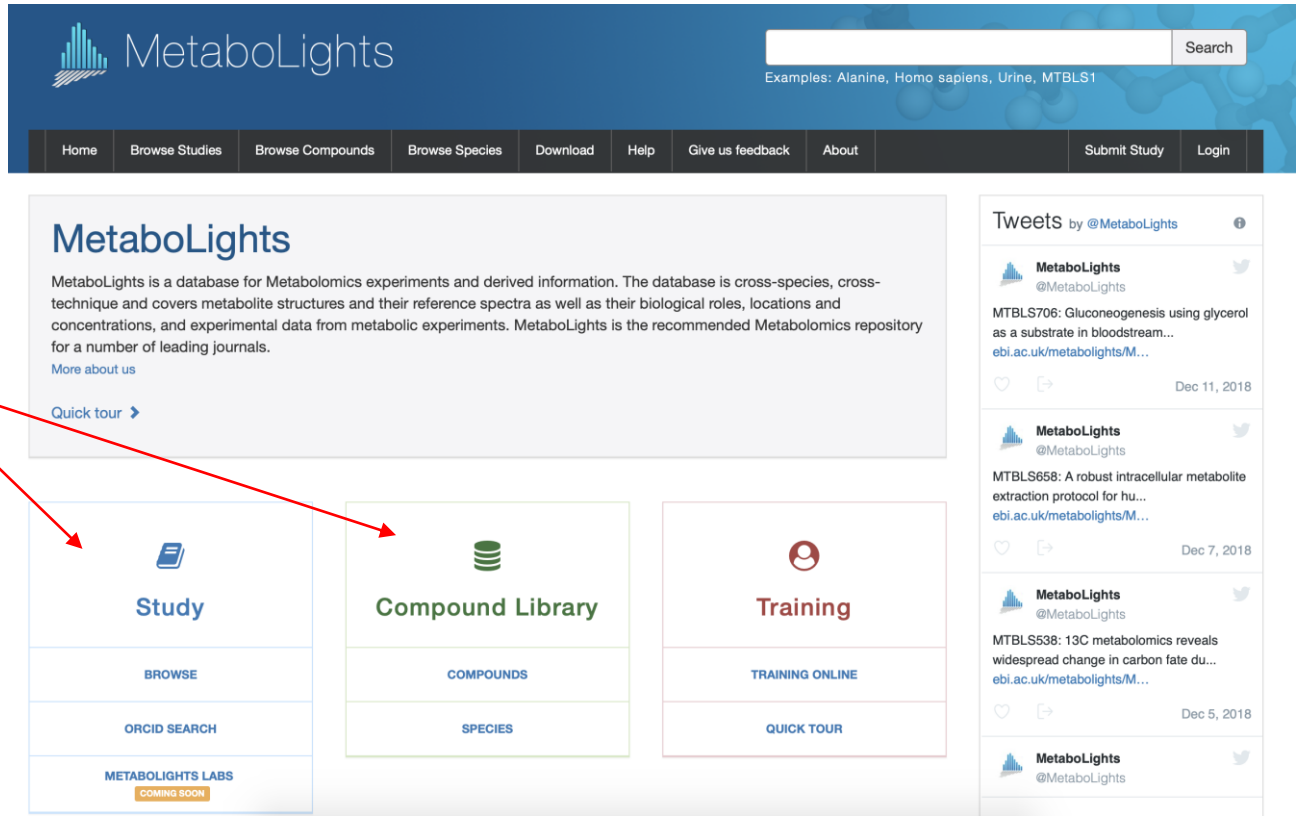


Repositories

VMH
VIRTUAL METABOLIC HUMAN

MetaboLights

Open Source Study Repository & Metabolite Knowledgebase



https://www.ebi.ac.uk/metabolights

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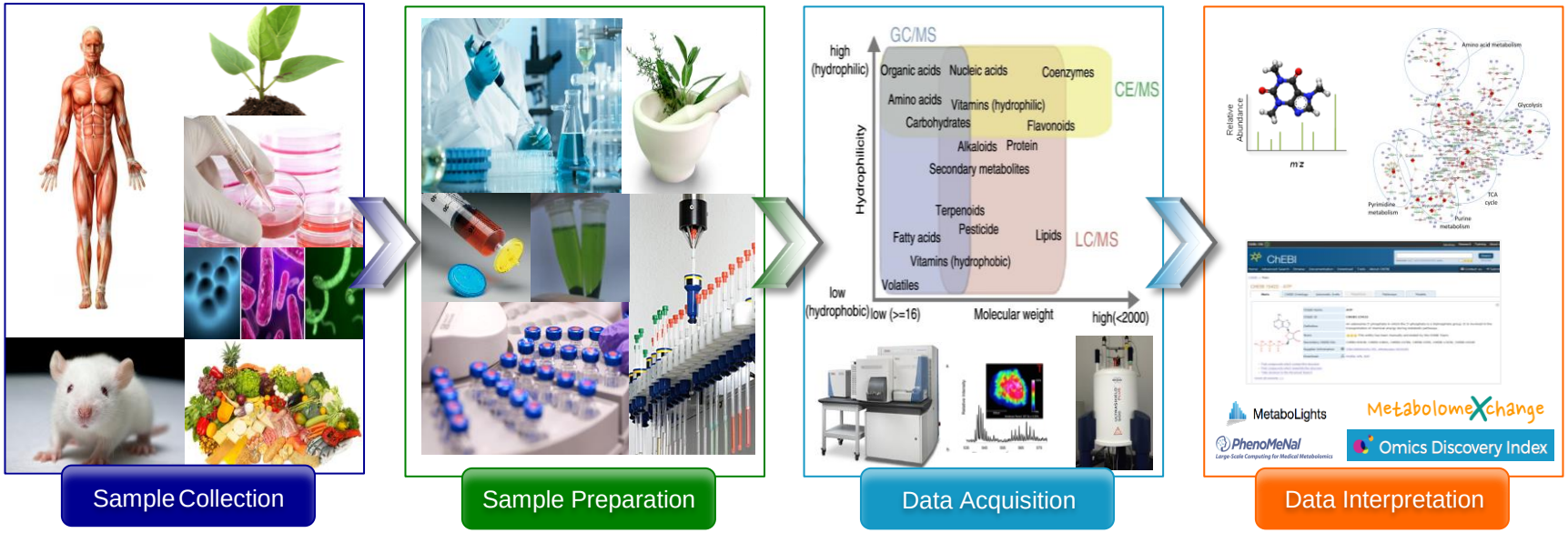
MetaboLights Database

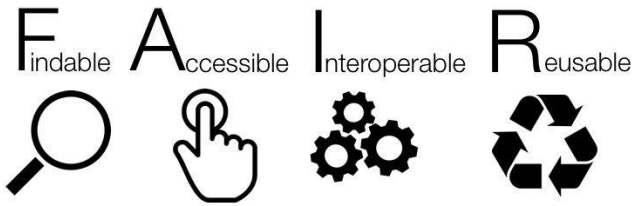


- Cross species, cross technique
- Comprehensive information collection
- Open access, discoverable through various portals

MetaboLights: Reporting standards

The Metabolomics Standards Initiative (MSI)

http://metabolomicssociety.org/



https://www.force11.org/group/fairgroup/fairprinciples

SCIENTIFIC DATA

PLOS BIOLOGY

METABOLOMICS

metabolites
an Open Access Journal by MDPI

frontiers

EMBL-EBI

https://www.ebi.ac.uk/submission/

The MetaboLights database was developed in conjunction with the metabolomics community to create a resource which aligned with community standards.

The primary requirement for a MetaboLights study submission is raw data. This is supported with rich metadata describing the samples and protocols, underpinned with controlled vocabularies / ontologies and unique identifiers. Together this represents many of the attributes of good data management as outlined in the FAIR principles.

Many funding bodies and journals require the submission of raw data to a public repository and MetaboLights is the recommended metabolomics resource for many.

It is also possible to link cross-omic data submissions through the EMBL-EBI genomics, transcriptomics and proteomics repositories.

MetaboLights user base

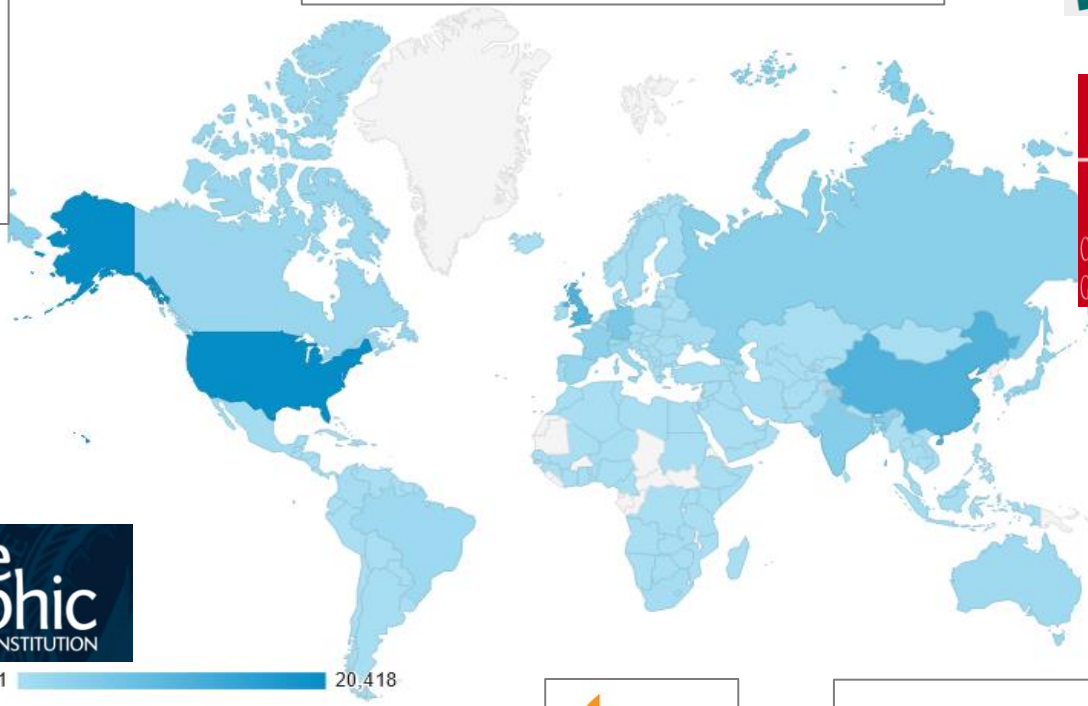
MaHPIC

Malaria Host-Pathogen Interaction Center (NIH)

METABOLON

Precision Metabolomics

MAX-PLANCK



OIST

OKINAWA INSTITUTE OF SCIENCE AND TECHNOLOGY GRADUATE UNIVERSITY

Pacific Northwest NATIONAL LABORATORY

NHS National Institute for Health Research BioResource

Woods Hole Oceanographic INSTITUTION

CHEAR Children's Health Exposure Analysis Resource

NIH

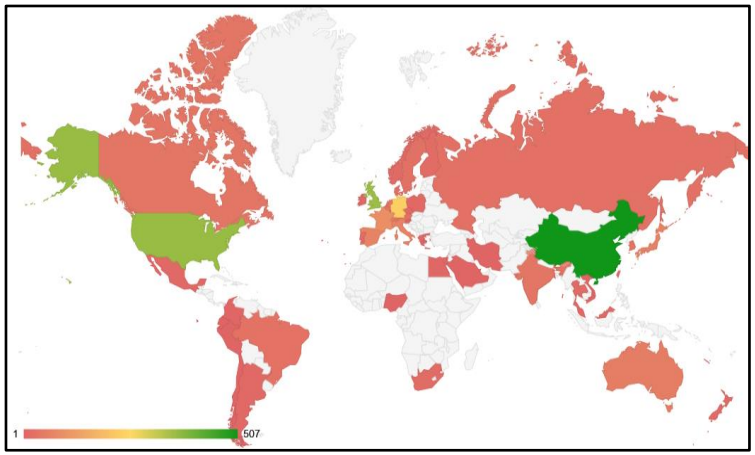
PHENOME CENTRE BIRMINGHAM

UNIVERSITY OF CAMBRIDGE

National Phenome Centre

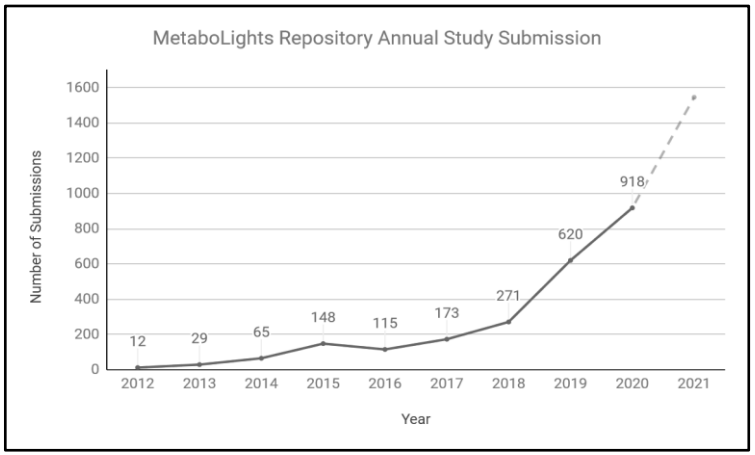
embric

EUROPEAN MARINE BIOLOGICAL RESEARCH INFRASTRUCTURE CLUSTER

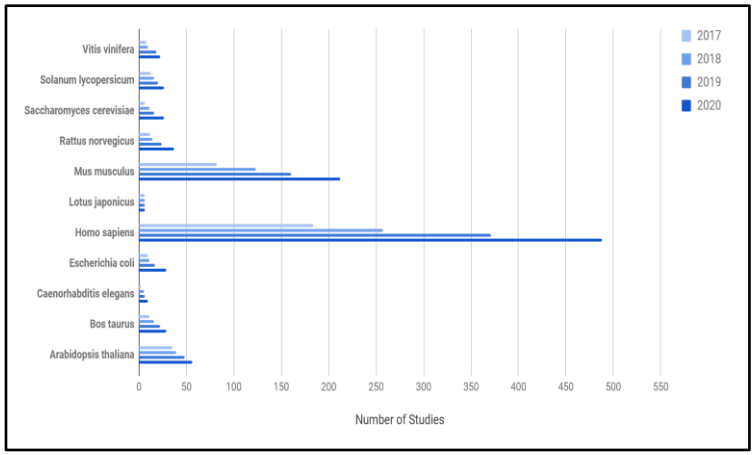


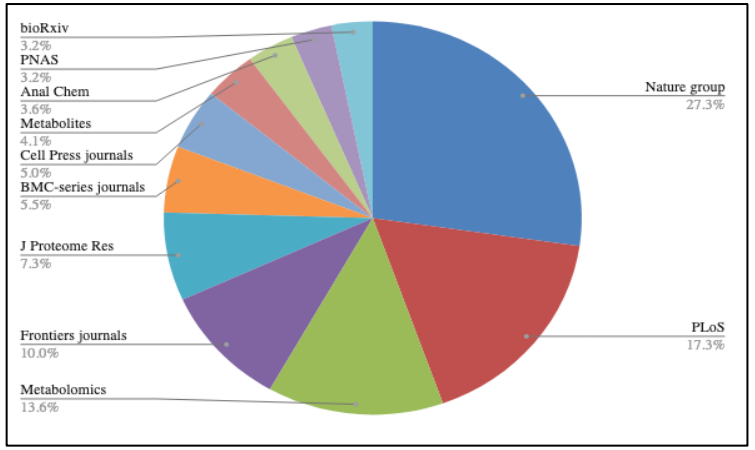
Geographical distribution of submitted studies

(Top 10: China: 507, USA: 362, UK: 356, Germany: 235, France: 94, Japan: 68, Spain: 66, Italy: 64, Australia: 53, Netherlands: 39)

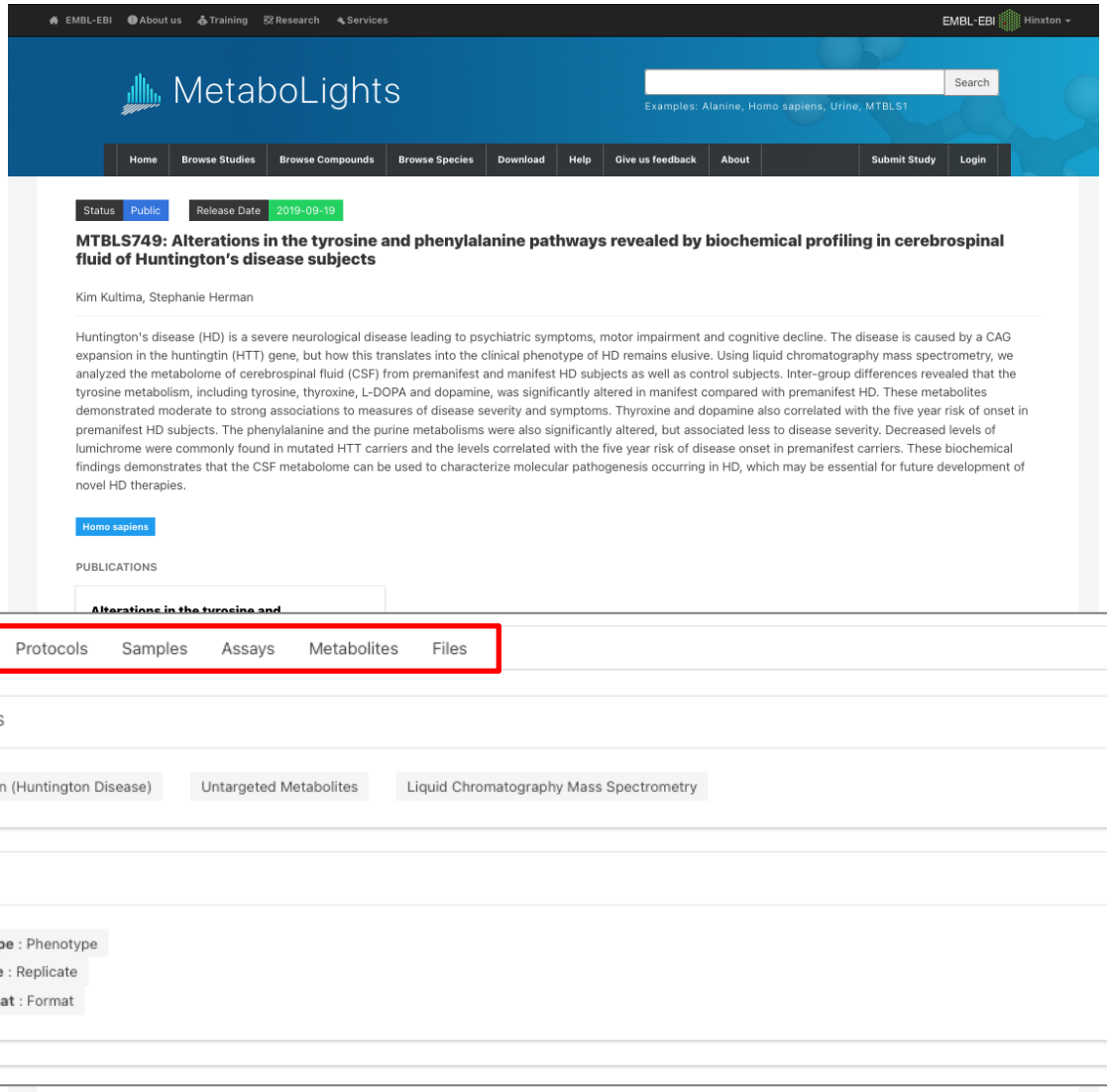


MetaboLights study submission rates per year





MetaboLights – Study information



MetaboLights Study Submission

MetaboLights

Individual researcher

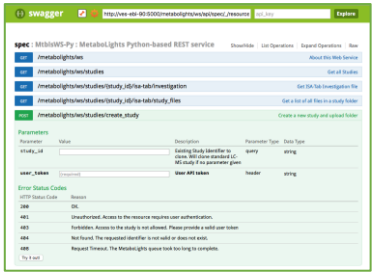
Labs
Phenome Centers

Industry
Metabolon etc.

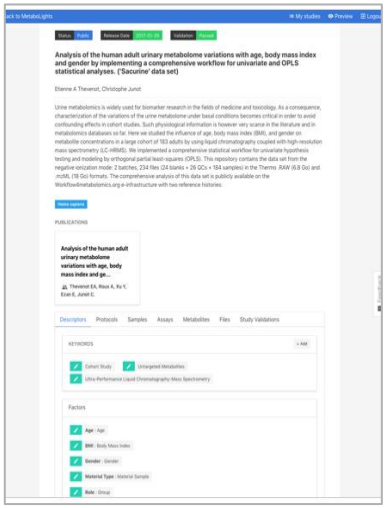
Online guided submission

Pipeline Template

REST API - Access



Online Editor



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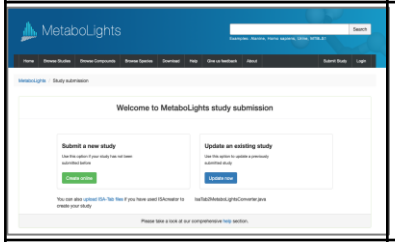
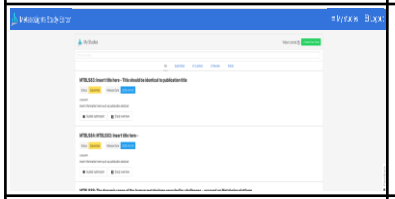
MetaboLights: Quickstart guide

Create account		To submit a study, first create an account with MetaboLights www.ebi.ac.uk/metabolights/login
Create new study		Select Submit study to create a new study. Create online: step by step guide, recommended option for submission. API option also available. NB. the unique accession number assigned to your study ***MTBLS…*** will be the final reference, please use this in manuscripts. *NB. For journal editor reviewer link see information below.*
Edit study online		If you don't have all the information available when creating your study, don't worry. Once the initial study has been created you can use the online editor option to add, edit and upload data. Access through your My Studies page.
Study curation process		Once the validation criteria has been met, change 'Status' to move study into the curation queue. NB. this process can take at least 4 weeks.
Private study link available for reviewers		Following completion of the curation process the status will be updated to review and a private link to your study will be available for you to share with journal editors etc.
Study publication		Curated studies will become public once the date you have set is reached. You can update this at any stage by contacting us directly metabolights-help@ebi.ac.uk

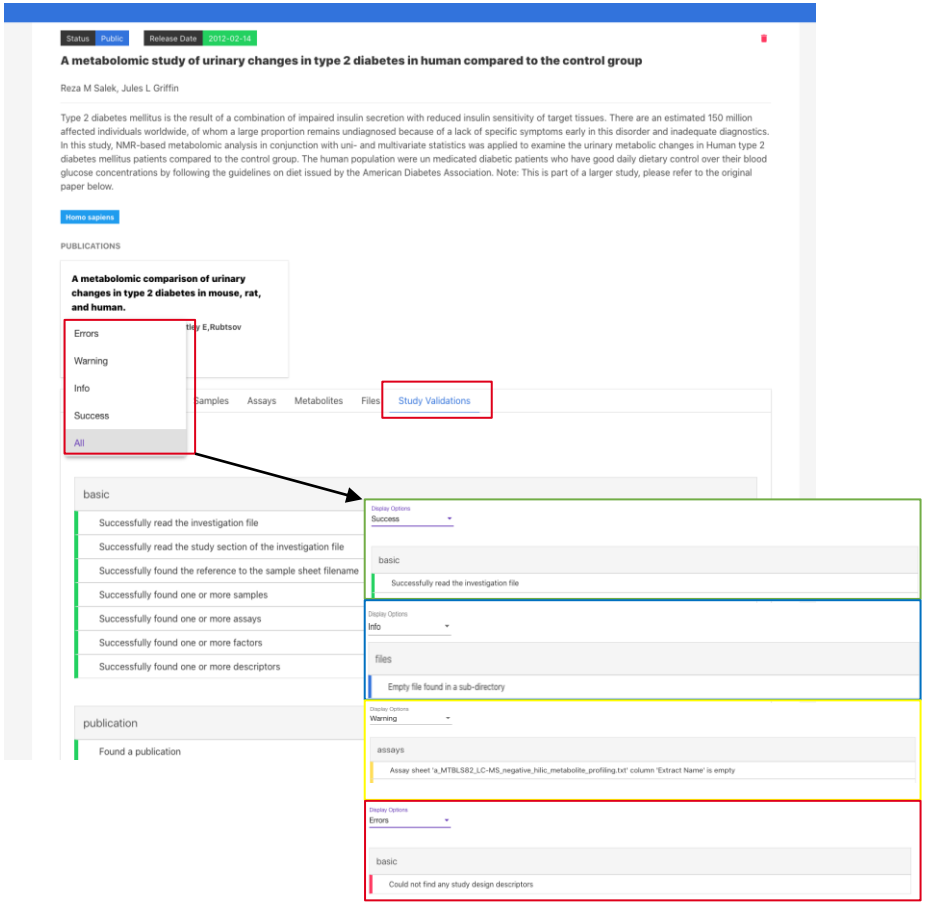
MetaboLights: Study completion

The publication of your study is in your control, however there are some factors to remember!

Validation Failed

You must ensure your study passes all the required validations. If the study displays **'Failed'**, please look at the study validations tab to find out more.
All '**Errors**' must be addressed to progress the study. '**Warning**' can help to alert you to missing or mismatched information.

The validation box will disappear when all validations are successful.



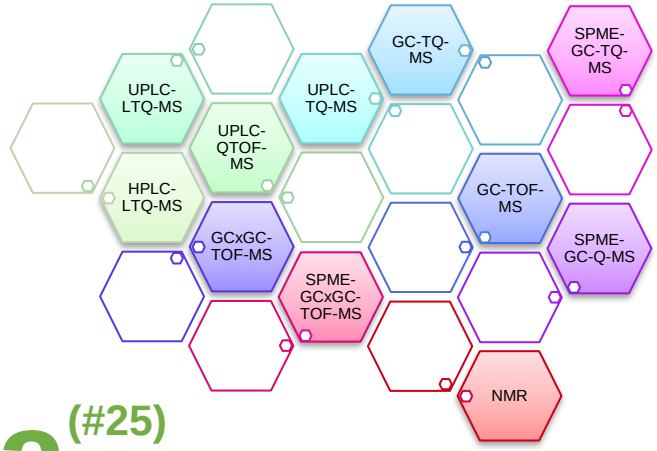
MetaboLights: Studies with Vitis

MetaboLights

3821 samples

16,682 metabolites

184 Gb

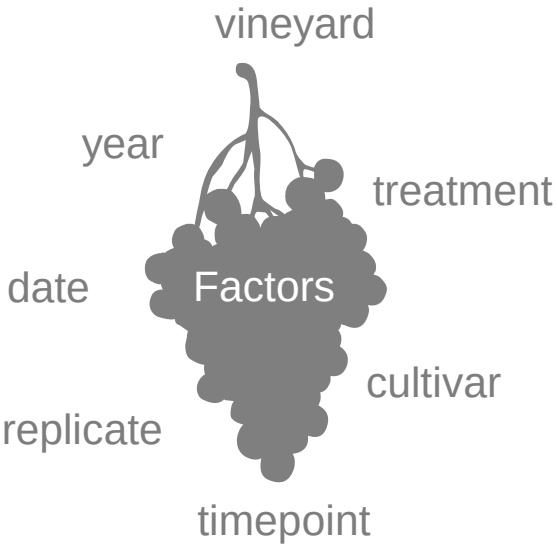


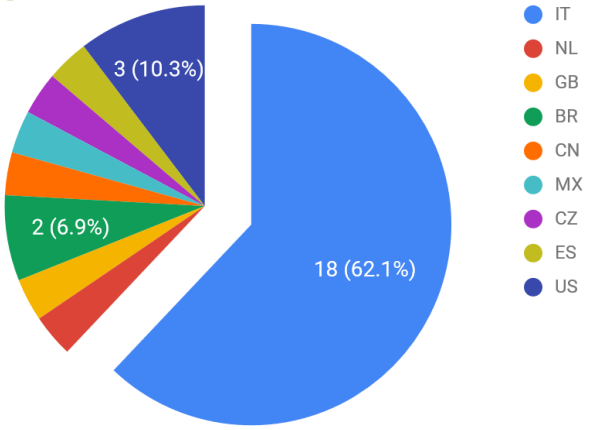
vitis labrusca(#2)

vitis vinifera(#25)

Vitis(#29)

vitis rotundifolia(#2)





number of studies in MetaboLights (prep to public)

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Acknowledgements

EMBL-EBI Metabolomics team

- Claire O'Donovan (PI)
- Pamela Pruski
- Mark Williams
- Felix Amaladoss
- Callum Martin
- Thomas Payne

The Metabolomics team's activities were supported in the past year by the above funding bodies

MetaboLights – Welcoming feedback!

User input on existing and new features

- Any features you would like to see included?
- How to best capture assay and metabolite annotations?
- What other kind of data would you like us to capture?
- What interactions with other resources would you like to see?

Email us **metabolights-help@ebi.ac.uk**