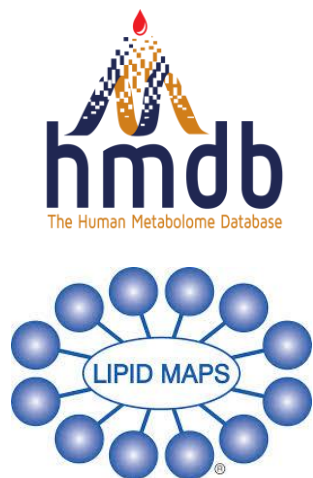


An introduction to MetaboLights

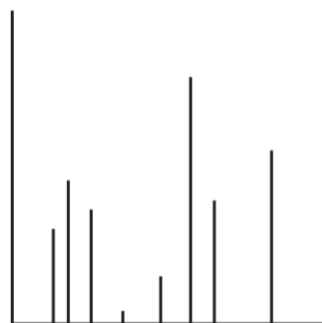
EMBL-EBI Metabolomics Team

www.ebi.ac.uk

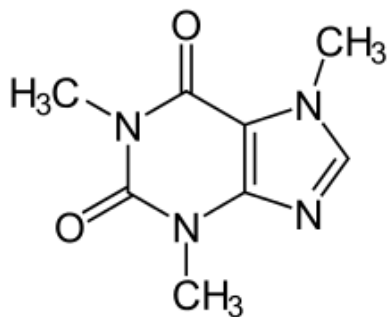
Metabolomics Resources



Spectral Libraries



Metabolite Knowledgebases



Analysis Tools



Repositories





Open Source Study Repository & Metabolite Knowledgebase

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.

[More about us](#)

[Quick tour >](#)

Study

BROWSE

ORCID SEARCH

METABOLIGHTS LABS
COMING SOON

Compound Library

COMPOUNDS

SPECIES

Training

TRAINING ONLINE

QUICK TOUR

Tweets by @MetaboLights

MetaboLights
@MetaboLights

MTBLS706: Gluconeogenesis using glycerol as a substrate in bloodstream...
ebi.ac.uk/metabolights/M...

Dec 11, 2018

MetaboLights
@MetaboLights

MTBLS658: A robust intracellular metabolite extraction protocol for hu...
ebi.ac.uk/metabolights/M...

Dec 7, 2018

MetaboLights
@MetaboLights

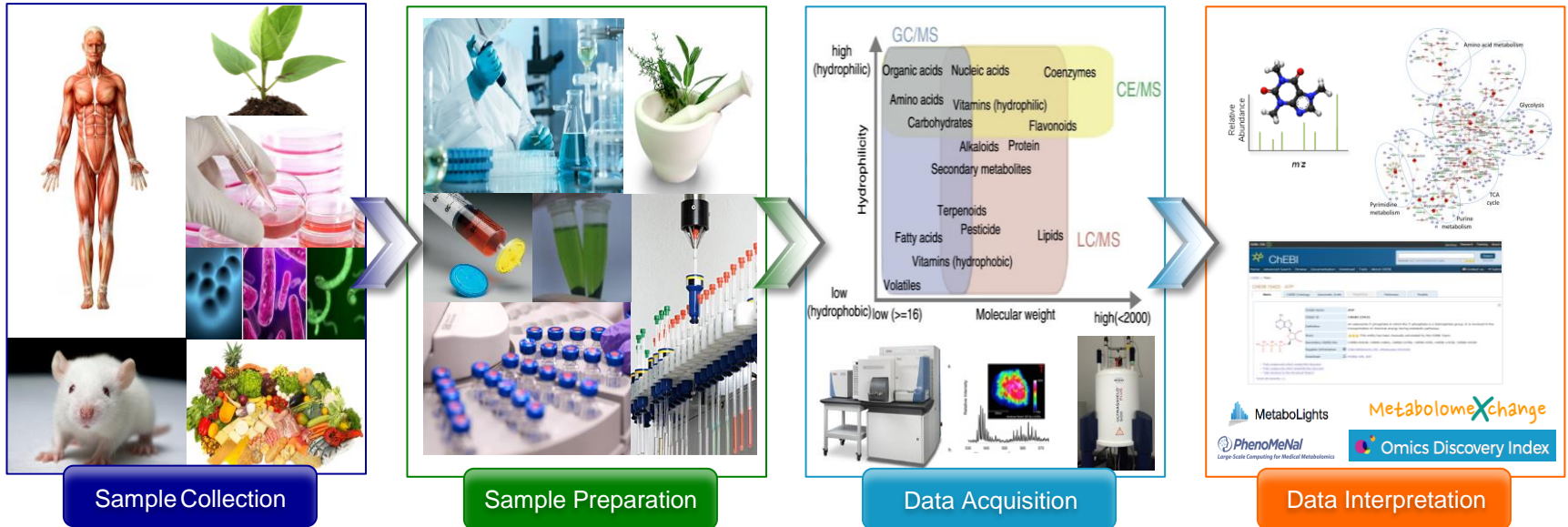
MTBLS538: 13C metabolomics reveals widespread change in carbon fate du...
ebi.ac.uk/metabolights/M...

Dec 5, 2018

MetaboLights
@MetaboLights

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

MetaboLights Database



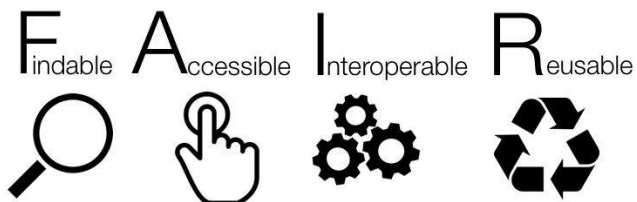
- Cross species, cross technique
- Comprehensive information collection
- Open access, discoverable through various portals

MetaboLights: Reporting standards



The Metabolomics Standards Initiative (MSI)

<http://metabolomicssociety.org/>



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

SCIENTIFIC DATA



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

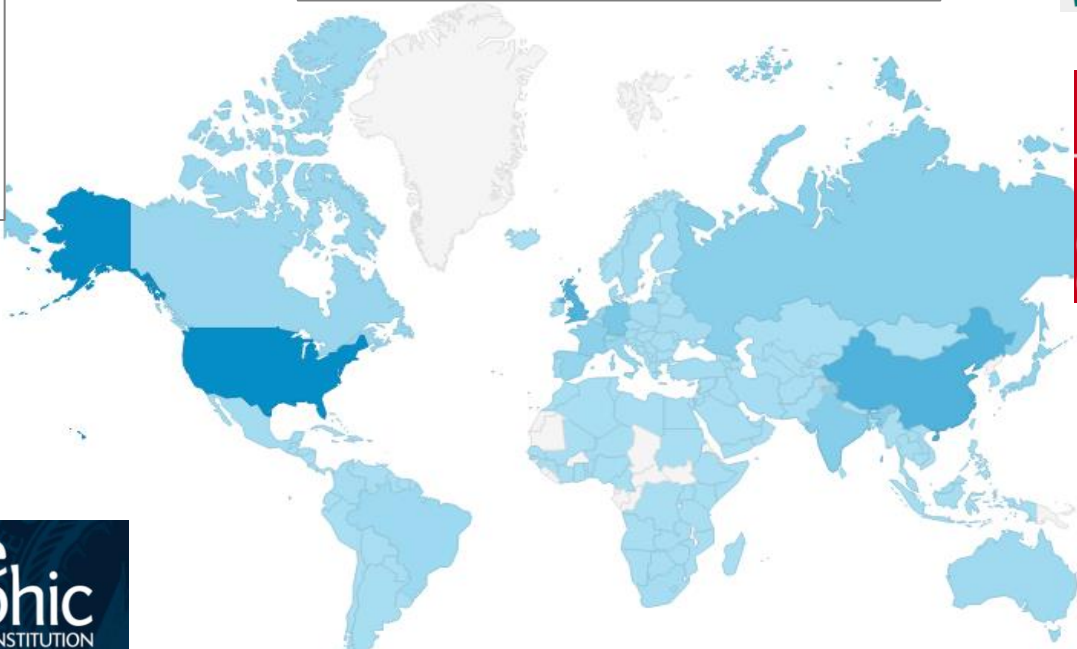
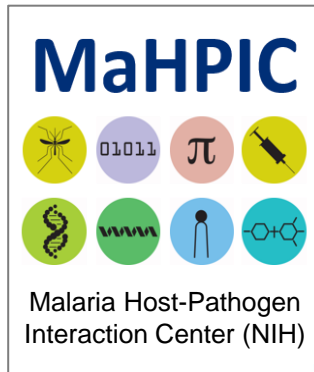
The MetaboLights database was developed in conjunction with the metabolomics community to create a resource which aligned with community standards.

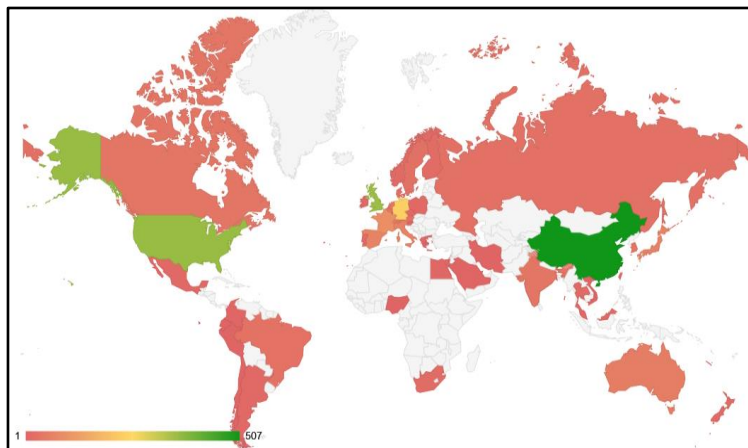
The primary requirement for a MetaboLights study submission is raw data. This is supported with rich metadata describing the samples and protocols, underpinned with controlled vocabularies / ontologies and unique identifiers. Together this represents many of the attributes of good data management as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

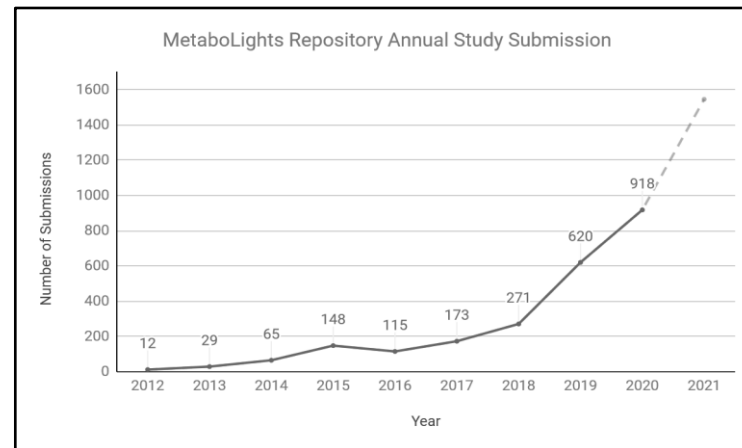
MetaboLights user base



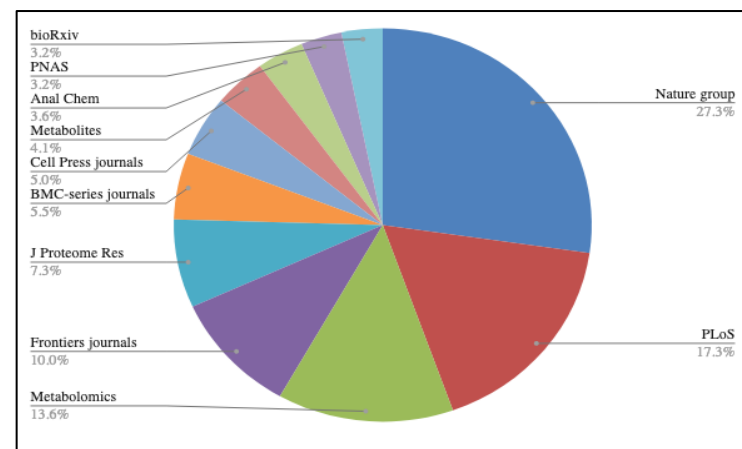
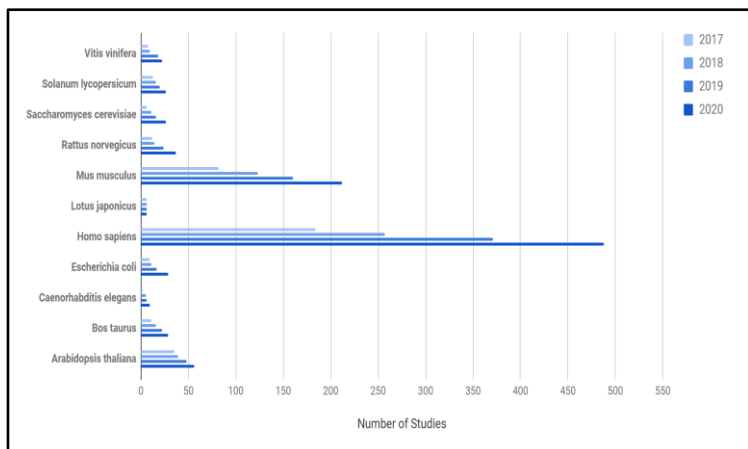


Geographical distribution of submitted studies

(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

The image shows the MetaboLights website interface. At the top, there is a navigation bar with links for Home, Browse Studies, Browse Compounds, Browse Species, Download, Help, Give us feedback, About, Submit Study, and Login. Below this is a search bar with the text "Examples: Alanine, Homo sapiens, Urine, MTBLS1". The main content area displays the study title "MTBLS749: Alterations in the tyrosine and phenylalanine pathways revealed by biochemical profiling in cerebrospinal fluid of Huntington's disease subjects" by Kim Kultima, Stephanie Herman. The study is marked as "Public" and has a release date of "2019-09-19". The abstract text describes the study's findings on the metabolome of cerebrospinal fluid (CSF) from premanifest and manifest HD subjects, highlighting alterations in tyrosine metabolism, thyroxine, L-DOPA, and dopamine, and their associations with disease severity and symptoms.

EMBL-EBI About us Training Research Services EMBL-EBI Hinxton

MetaboLights

Search

Examples: Alanine, Homo sapiens, Urine, MTBLS1

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

Status **Public** Release Date **2019-09-19**

MTBLS749: Alterations in the tyrosine and phenylalanine pathways revealed by biochemical profiling in cerebrospinal fluid of Huntington's disease subjects

Kim Kultima, Stephanie Herman

Huntington's disease (HD) is a severe neurological disease leading to psychiatric symptoms, motor impairment and cognitive decline. The disease is caused by a CAG expansion in the huntingtin (HTT) gene, but how this translates into the clinical phenotype of HD remains elusive. Using liquid chromatography mass spectrometry, we analyzed the metabolome of cerebrospinal fluid (CSF) from premanifest and manifest HD subjects as well as control subjects. Inter-group differences revealed that the tyrosine metabolism, including tyrosine, thyroxine, L-DOPA and dopamine, was significantly altered in manifest compared with premanifest HD. These metabolites demonstrated moderate to strong associations to measures of disease severity and symptoms. Thyroxine and dopamine also correlated with the five year risk of onset in premanifest HD subjects. The phenylalanine and the purine metabolisms were also significantly altered, but associated less to disease severity. Decreased levels of lumichrome were commonly found in mutated HTT carriers and the levels correlated with the five year risk of disease onset in premanifest carriers. These biochemical findings demonstrates that the CSF metabolome can be used to characterize molecular pathogenesis occurring in HD, which may be essential for future development of novel HD therapies.

Homo sapiens

PUBLICATIONS

Alterations in the tyrosine and

The image shows a sidebar for the study MTBLS749. The "Descriptors" tab is highlighted with a red box. Below the tabs, there are sections for KEYWORDS and Factors. The KEYWORDS section lists "Huntingtin (Huntington Disease)", "Untargeted Metabolites", and "Liquid Chromatography Mass Spectrometry". The Factors section lists "Phenotype : Phenotype", "Replicate : Replicate", and "MS Format : Format".

Descriptors Protocols Samples Assays Metabolites Files

KEYWORDS

Huntingtin (Huntington Disease) Untargeted Metabolites Liquid Chromatography Mass Spectrometry

Factors

Phenotype : Phenotype

Replicate : Replicate

MS Format : Format

MetaboLights Study Submission



MetaboLights



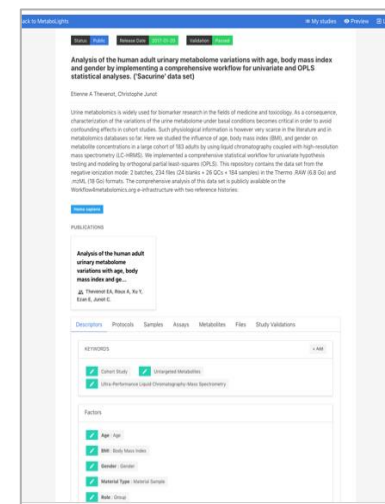
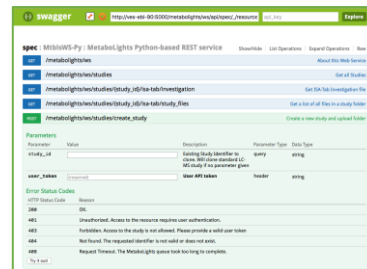
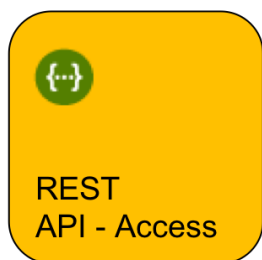
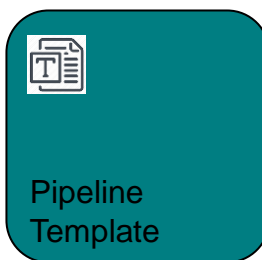
Individual researcher



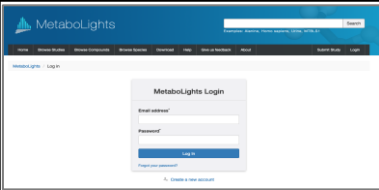
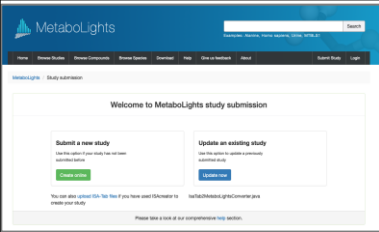
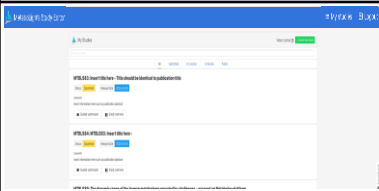


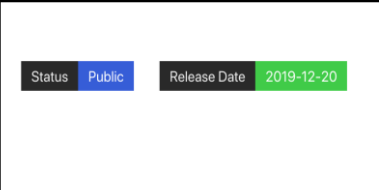
Labs
Phenome Centers



Industry
Metabolon etc.



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. <i>NB. For journal editor reviewer link see information below.</i>
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.

The screenshot displays the MetaboLights study completion interface. At the top, the status is 'Public' and the release date is '2012-02-14'. The study title is 'A metabolomic study of urinary changes in type 2 diabetes in human compared to the control group' by Reza M Salek, Jules L Griffin. The abstract describes a study on type 2 diabetes mellitus. The interface includes a 'Study Validations' tab, which is currently selected. A dropdown menu on the left shows the validation status: 'Errors' (highlighted in red), 'Warning', 'Info', 'Success', and 'All'. The main content area shows a list of validation results, categorized by 'basic', 'publication', and 'assays'. The 'basic' category shows several successful validations. The 'publication' category shows 'Found a publication'. The 'assays' category shows a warning: 'Assay sheet 'x_MTBLS82.LC-MS_negative_hsic_metabolite_profiling.txt' column 'Extract Name' is empty'. The 'Errors' category shows a message: 'Could not find any study design descriptors'.

3821
samples



16,682
metabolites

184 Gb

vitis labrusca^(#2)

vitis vinifera^(#25)

Vitis^(#29)

vitis rotundifolia^(#2)

vineyard

year

treatment

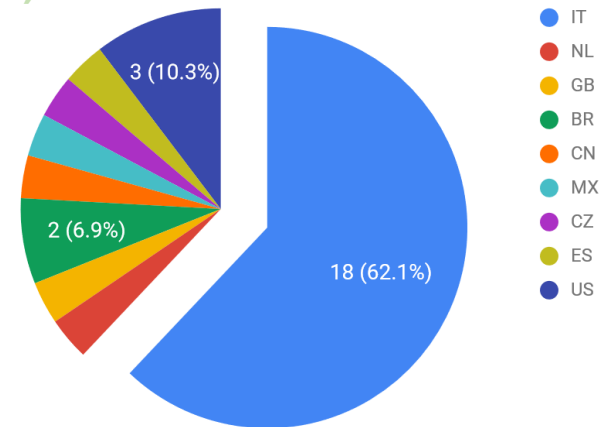
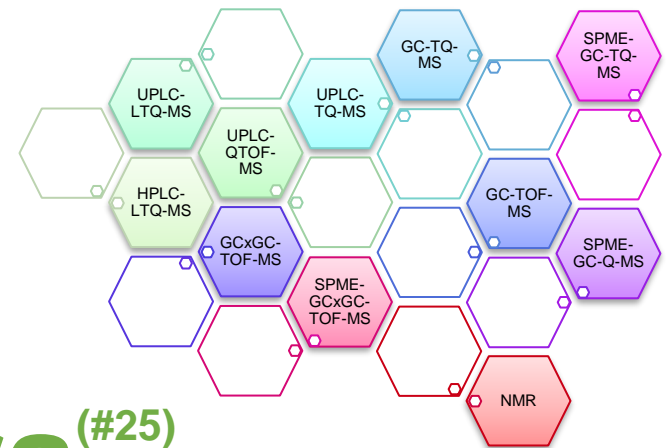
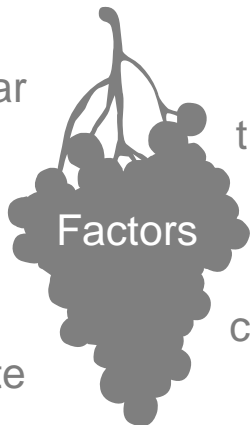
date

Factors

cultivar

replicate

timepoint



number of studies in MetaboLights (prep to public)

Acknowledgements

EMBL-EBI Metabolomics team

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



Horizon 2020

wellcome^{trust}

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**