

# Data Sharing, Standards and workflows in Metabolomics: Towards reproducible Metabolomics

Reza Salek PhD

Metabolism and Molecular Informatics

The European Bioinformatics Institute (EMBL-EBI)

Email: [Reza.salek@ebi.ac.uk](mailto:Reza.salek@ebi.ac.uk)

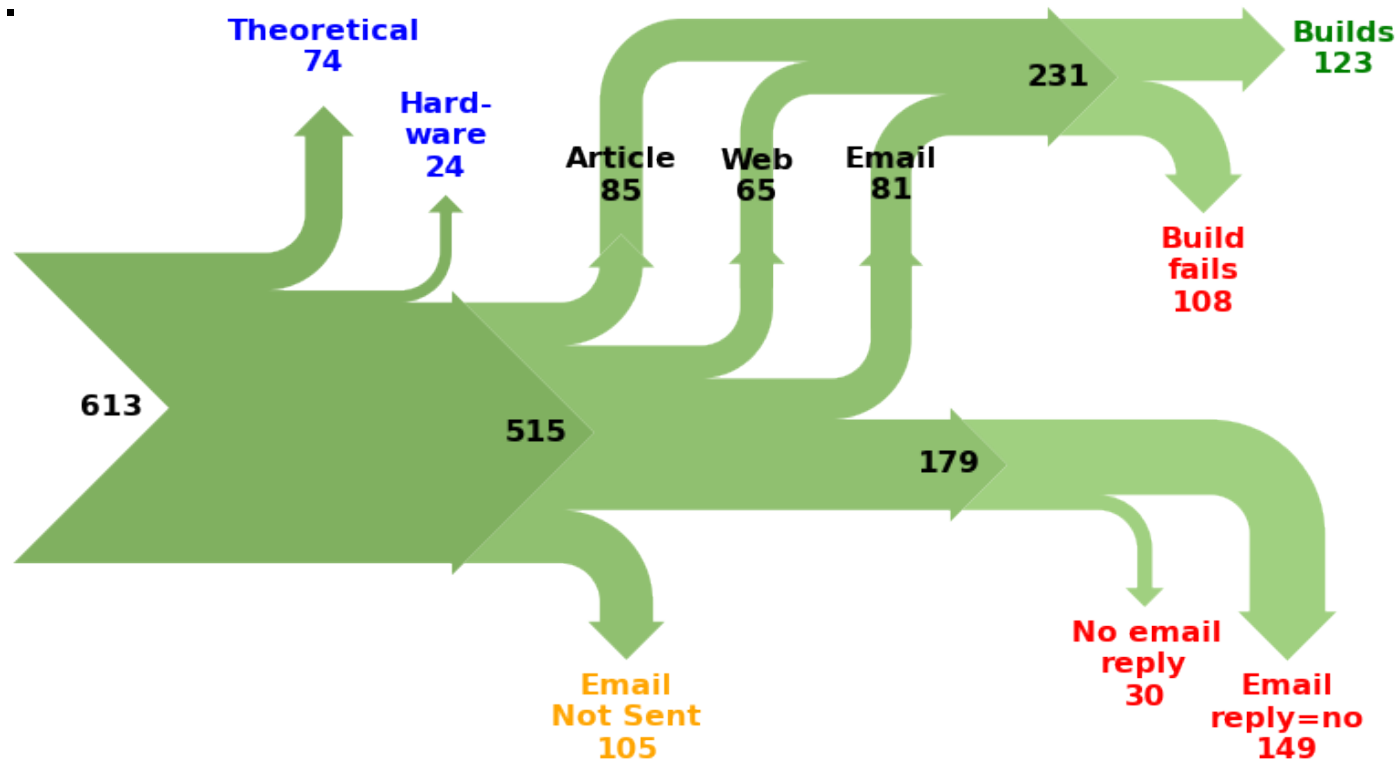
**NETTAB Rome 2016**

# To make efficient use of data...

- What do I mean by reproducibility
- Data Sharing;
  - – data publication is insufficient
  - – data “sharing” is needed for reuse, mashup, and integration of the data
- Standards;
  - – **standardization** of terminology – MI and SOP
    - via Society or international organizations
  - – standardization of **data exchange** format
  - – **clarification of rules** regarding data exchange (copyright, personal information, etc...)
  - – **Privacy and ethic** were applicable
- Creation and management of a **portal website** from which users access existing DB
  - Data analysis reproducibility

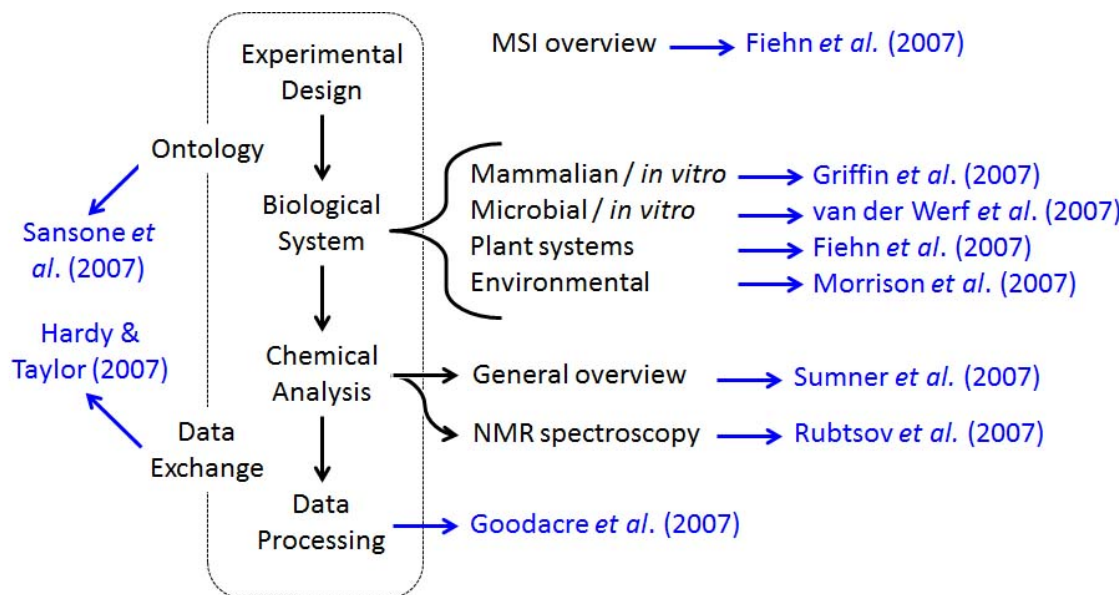
# Example: Digital! Reproducibility

Reproducibility is a **cornerstone of the scientific** process: only if my colleagues can reproduce my work should they trust its veracity.



# Metabolomics Standard Initiative (WG)

- Lives at <http://msi-workgroups.sourceforge.net>
- 5 Workgroups
  - Biological context metadata WG
  - Chemical analysis WG
  - Data processing WG
  - Ontology WG
  - Exchange format WG

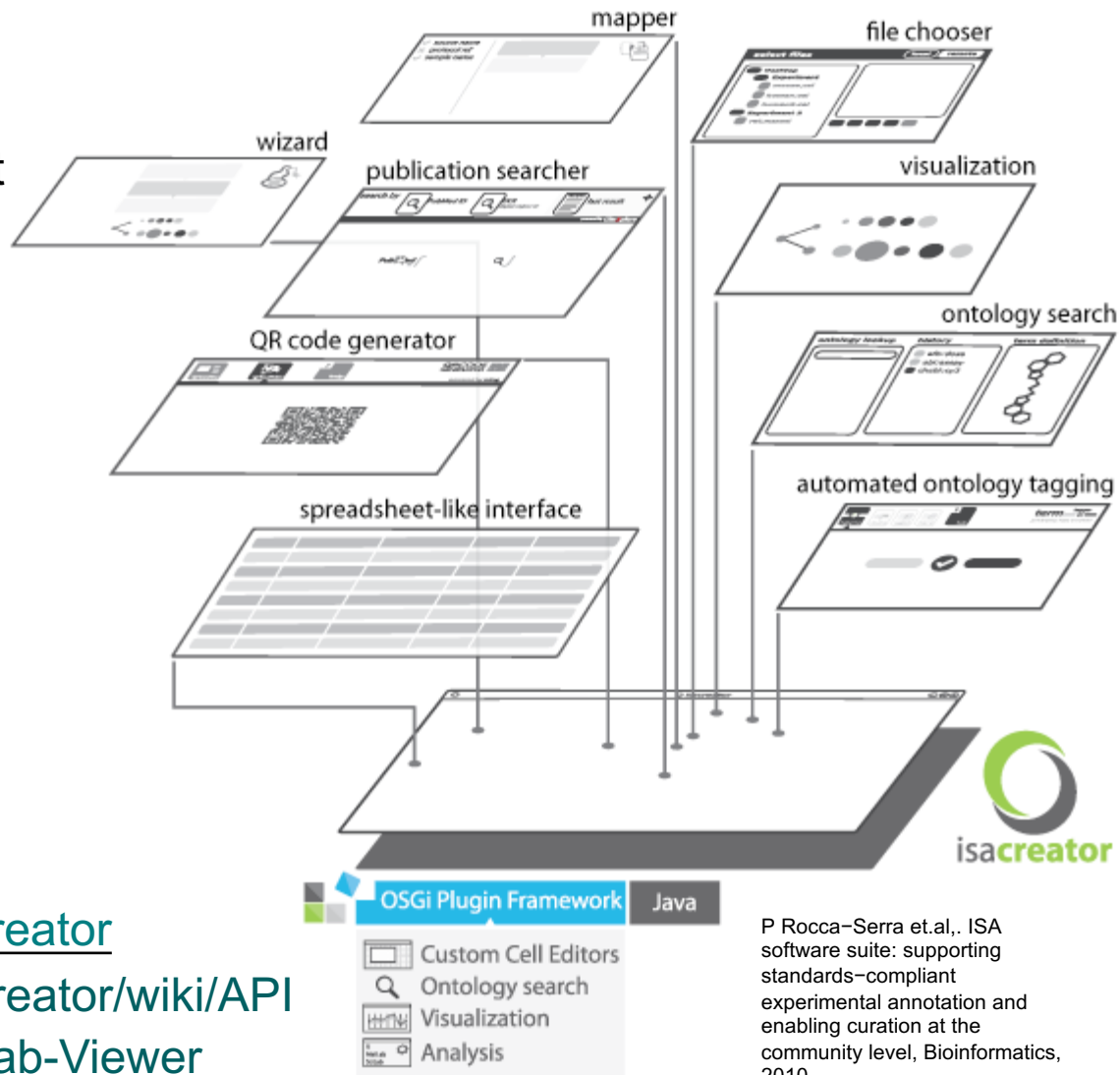


Roy Goodacre Metabolomics (2014) 10:5-7



# Capturing Metadata: ISA-Tab format

Developed a user friendly way to capture standards-compliant metadata



P Rocca-Serra et.al., ISA software suite: supporting standards-compliant experimental annotation and enabling curation at the community level, Bioinformatics, 2010.

<https://github.com/ISA-tools/ISAcreeator>

<https://github.com/ISA-tools/ISAcreeator/wiki/API>

<https://github.com/ISA-tools/ISATab-Viewer>

# ISAcreeator – Using Ontologies

search ontologies

browse suggested ontologies

view history

term definition

☒ Recommended Ontologies

☐ All Ontologies

Search for: 

search

4 terms from 2 ontologies

☒ NCBITaxon - NCBI organismal classification

Caenorhabditis elegans(obo:NCBITaxon\_6239)

Caenorhabditis elegans/Monacrosporium haptotylum mixed EST library(obo:NCBITaxon\_6239)

☒ NEWT - NEWT UniProt Taxonomy Database

filter

Term name: Caenorhabditis elegans

Service Provider: BioPortal

accession: obo:NCBITaxon\_6239

database\_cross\_reference: GC\_ID:1

has\_exact\_synonym: nematode

has\_obo\_namespace: ncbi\_taxonomy

has\_related\_synonym: Rhabditis elegans

oboInOwl:id: NCBITaxon:6239

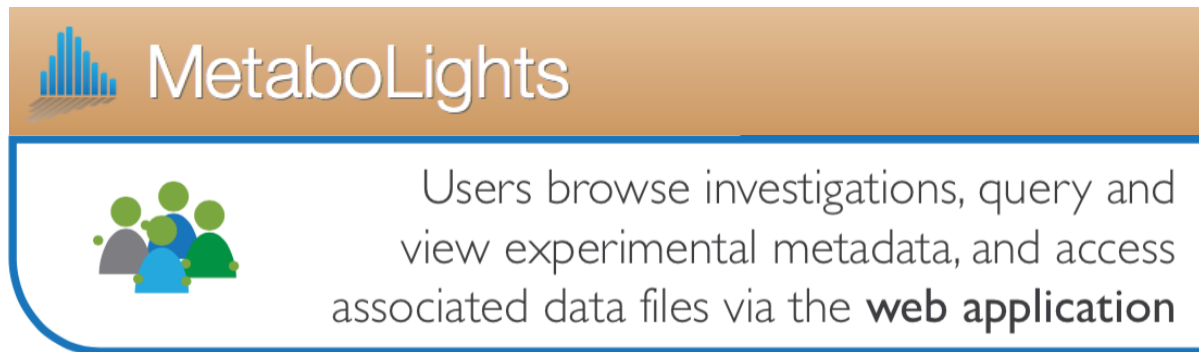
rdfs:label: Caenorhabditis elegans

Selected term. (You can also enter freetext here):

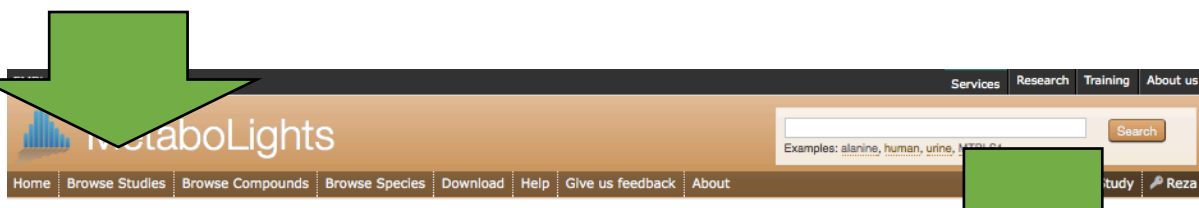
# MetaboLights – Current submission pipeline



Share private prepublication studies with reviewers and other trusted parties.



# MetaboLights Studies and Compounds



You are browsing MetaboLights

Filter your results

Privacy

- ☐ Private studies
- ☐ Public studies

Organism

Find your Organism

- ☐ Aedes albopictus
- ☐ Alluropoda melanoleuca
- ☐ Alkane standard
- ☐ Arabidopsis (ecotype Wassilewskija, Ws)
- ☐ Arabidopsis thaliana
- ☐ Arabidopsis thaliana (thale cress)
- ☐ Astragalus mongholicus
- ☐ Bacillus methanolicus
- ☐ Bacillus subtilis
- ☐ biofilm
- ☐ blank
- ☐ Blank
- ☐ blank value
- ☐ Bos Taurus
- ☐ Bos taurus (Bovine)
- ☐ Bovinae
- ☐ C57BL/6
- ☐ Caenorhabditis elegans
- ☐ Calanus helgolandicus (Copepod)
- ☐ Calibrator
- ☐ cell culture
- ☐ ...

Technology

- ☐ mass spectrometry
- ☐ NMR spectroscopy

195 Search result(s) showing 11 to 20

**Wax ester and lipophilic compound profiling of *Euglena gracilis* by gas chromatography-mass spectrometry: toward understanding of anoxia wax ester fermentation**  
Release date: 04-Sep-2014

Organism

- ☐ Euglena
- ☐ reference compound

Study Factors

- ☐ Culture days before anoxia incubation: [NA day, 4 day:2 day]
- ☐ Temperature: [27 degree Celsius:28 degree Celsius, NA degree Celsius]
- ☐ Anoxia incubation time: [24 hour:0 hour:4 hour, NA hour]
- ☐ Euglena strain: [wild type (Z strain):Bleached mutant (SM-ZK strain), Stand...
- ☐ Color: [Green:Orange, NA]
- ☐ Carbonate addition: [Present:none, none]

Assay

- ☐ mass spectrometry (114)

**NMR-based Blood Metabolic Profiles of Rats Exposed to Different Levels of ...**  
Release date: 05-Sep-2014

Organism

- ☐ Wistar Rat

Study Factors

- ☐ Caloric restriction: [40 %, 20 %, 0 %]

Assay

- ☐ NMR spectroscopy (15)

MetaboLights > Compound search

17487 RESULTS FOUND

Page : 1 Showing results 1 to 10 1 2 3 4 5 ... 1749 ▶

**Study status**

- ☐ Public
- ☐ Private

**Technology**

- ☐ NMR spectroscopy
- ☐ mass spectrometry
- ☐ not reported

**Organism**

- ☐ Aaptos oiliata
- ☐ Abacopteris penangiana
- ☐ Abelmoschus esculentus
- ☐ Abrus precatorius
- ☐ Acacia aulacocarpa
- ☐ Acacia jacquemontii
- ☐ Acacia meamii
- ☐ Acacia mellifera
- ☐ Acacia pennata
- ☐ Acacia schaffneri
- ☐ Acalypha indica

**(-)-beta-santalene (MTBLC10440)**

A sesquiterpene and carbobicyclic compound that is bicyclo[2.2.1]heptane in which the hydrogens at position 3 are substituted by a methylenedio group, while the 2-exo- and 2-endo- hydrogens are substituted by 2-methylpent-2-en-5-yl and methyl groups, respectively (the 1S,2R,4R enantiomer).

**3-methyl-2-oxobutanoic acid (MTBLC16530)**

A 2-oxo monocarboxylic acid that is the 2-oxo derivative of isovaleric acid.

Identified in [MTBLS1](#), [MTBLS222](#), [MTBLS48](#), [MTBLS49](#)

**L-sorbose (MTBLC17266)**

The L enantiomer of sorbose, a ketone-containing hexose (a six-carbon monosaccharide).

Currently No Image

MetaboLights - an open-access general-purpose repository for metabolomics studies and associated meta-data. *Nucl. Acids Res.* (2012) doi:10.1093/nar/gks1004

# MetaboLights – Study Validation Status

EMBL-EBI

Services Research Training About us

## MetaboLights

MTBLS1  
Examples: alanine, human, urine, MTBLS1

Search

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

Submit Study Login

MetaboLights > Search

### You are searching MetaboLights

+ Show more data from EMBL-EBI

Filter your results

Type

- ☐ compound
- ☐ study

Organism

Find your Organism

- ☐ Homo sapiens
- ☐ Daphnia magna
- ☐ Saccharomyces cerevisiae
- ☐ reference compound
- ☐ Caenorhabditis elegans
- ☐ Schizosaccharomyces pombe 972h-
- ☐ Arabidopsis thaliana

52 results, showing 1 to 10

Page 1 of 6

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

**Validations Status:** ○ ○ ●

**Release date:** 14-Feb-2012

**Organism**

- Homo sapiens

**Study Factors**

- Gender
- Metabolic syndrome

Study identifier: **MTBLS1**  
Total Study size: **229.97MB**  
Submitted by  
Reza Salek

# MetaboLights – Study Validation details

[Study Design Description](#) [Protocols](#) [Samples](#) [Assay ▾](#) [Study Files](#) [Study Validation ✖](#)

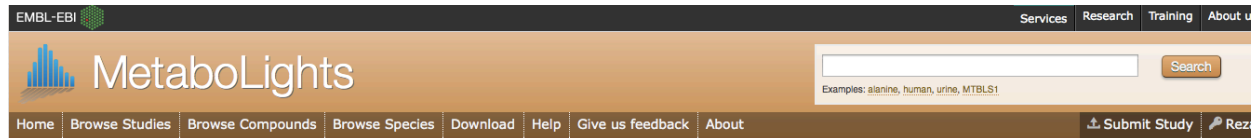
Validations marked with (\*) are specially approved by the MetaboLights Curators

Show  entries Search:

Condition ▴▾	Status ▴▾	Description ▴▾	Requirement ▴▾	Group ▴▾	Message ▴▾
✓	PASSES	Study Title	MANDATORY	STUDY	OK
✓	PASSES	Study Description	MANDATORY	STUDY	OK
✓	PASSES	Study text successfully parsed	OPTIONAL	STUDY	OK
✓	PASSES	Study Contact(s) have listed email	MANDATORY	CONTACT	OK
✓	PASSES	Sample(s)	MANDATORY	SAMPLES	OK
✓	PASSES	Sample Name consistency check	MANDATORY	ASSAYS	OK
✖	FAILS	Publication(s) associated with this Study	MANDATORY	PUBLICATION	Study Publication is missing
✓	PASSES	Minimal Experimental protocol	MANDATORY	PROTOCOLS	OK
✖	INCOMPLETE	Comprehensive Experimental protocol	OPTIONAL	PROTOCOLS	Protocol description is not sufficiently detailed or not all required fields are provided. Missing field(s): Chromatography, Metabolite identification, Sample collection
✖	FAILS	Sample Collection protocol	MANDATORY	PROTOCOLS	Sample data is provided but no 'Sample collection' protocol is described

Showing 1 to 10 of 19 entries Previous **1** 2 Next

# Data sharing repositories



MetaboLights > Browse

You are browsing MetaboLights

Filter your results

Privacy

- ☐ Private studies
- ☐ Public studies

Organism

Find your Organism

- ☐ Alkane standard
- ☐ Arabidopsis (ecotype Wassilewskija, Ws)
- ☐ Arabidopsis thaliana.Col-0
- ☐ Arabidopsis thaliana (thale cress)
- ☐ biofilm
- ☐ Bos taurus (Bovine)
- ☐ Bovinae
- ☐ C57BL/6
- ☐ Caenorhabditis elegans
- ☐ Calanus helgolandicus
- ☐ Chlamydomonas reinhardtii
- ☐ HEK293
- ☐ Homo sapiens
- ☐ Homo sapiens (Human)
- ☐ Hordeum vulgare var. distichum (Two-rowed)

71 Search result(s) showing 1 to 10

1 2 3 4 5 6 7 8 ▶

NMR based metabolomics of Human Type 2 Diabetes urine samples

Release date: 15-Feb-2012

Organism

- Homo sapiens (Human)

Study Factors

- Metabolic syndrome: [type 2 diabetes mellitus:Control Group]
- Gender: [Female Gender(Female\_Gender):Male Gender(Male\_Gender)]

Assay

- NMR spectroscopy (132)

Metabolomics profile of herbivory-induced Nicotiana attenuata plants

Release date: 14-Aug-2012

Organism

- Nicotiana attenuata (Coyote tobacco)

<http://www.metabolomicsworkbench.org/>



Welcome to the UCSD Metabolomics Workbench, a resource sponsored by the Common Fund of the National Institutes of Health.

## Invitation to deposit metabolomics experimental data

The Metabolomics Workbench is now accepting metabolomics data from NIH grantees/projects, as long as the metadata and results requirements are followed. Templates for data deposition are available in the "Metadata and Experimental Data Deposition" [section](#) of the website along with tutorials and examples on the organization of the data infrastructure and use of these templates. For any questions concerning data upload please contact [Dr. Eoin Fahy](#).

## Invitation to Nominate Compounds for Synthesis

As part of the NIH Common Fund's Metabolomics Program, the Metabolite Standards Synthesis Core (MSSC) aims to provide metabolomics researchers with high quality metabolite standards. We invite scientists to [nominate compounds for synthesis](#). Nominated compounds will be reviewed by the NIH Common Fund's executive committee, and prioritized for synthesis.

## Metabolomics Workbench Highlights

Three new Regional Comprehensive Metabolomics Resource Cores (RCMRC)s have joined the NIH Metabolomics Consortium:

- [Southeast Center for Integrated Metabolomics \(SECIM\)](#)

## Funding Opportunities

[Call for Pilot and Feasibility Project Applications from Regional Comprehensive Metabolomics Research Cores](#)

## Regional Comprehensive Metabolomics Resource Cores (RCMRC)s

[Michigan Regional Comprehensive Metabolomics Resource Core \(MRC\)²](#)

[NIH West Coast Metabolomics Center at UC Davis](#)

[NIH Eastern Regional Comprehensive Metabolomics Resource Core at RTI International](#)

[Southeast Center for Integrated Metabolomics \(SECIM\)](#)

[Resource Center for Stable Isotope-Resolved Metabolomics \(RC-SIRM\)](#)

[Metabolomics Core at Mayo Clinic](#)

• [RCMRC press releases](#)

Format conversion

<http://ebi.ac.uk/metabolights/>

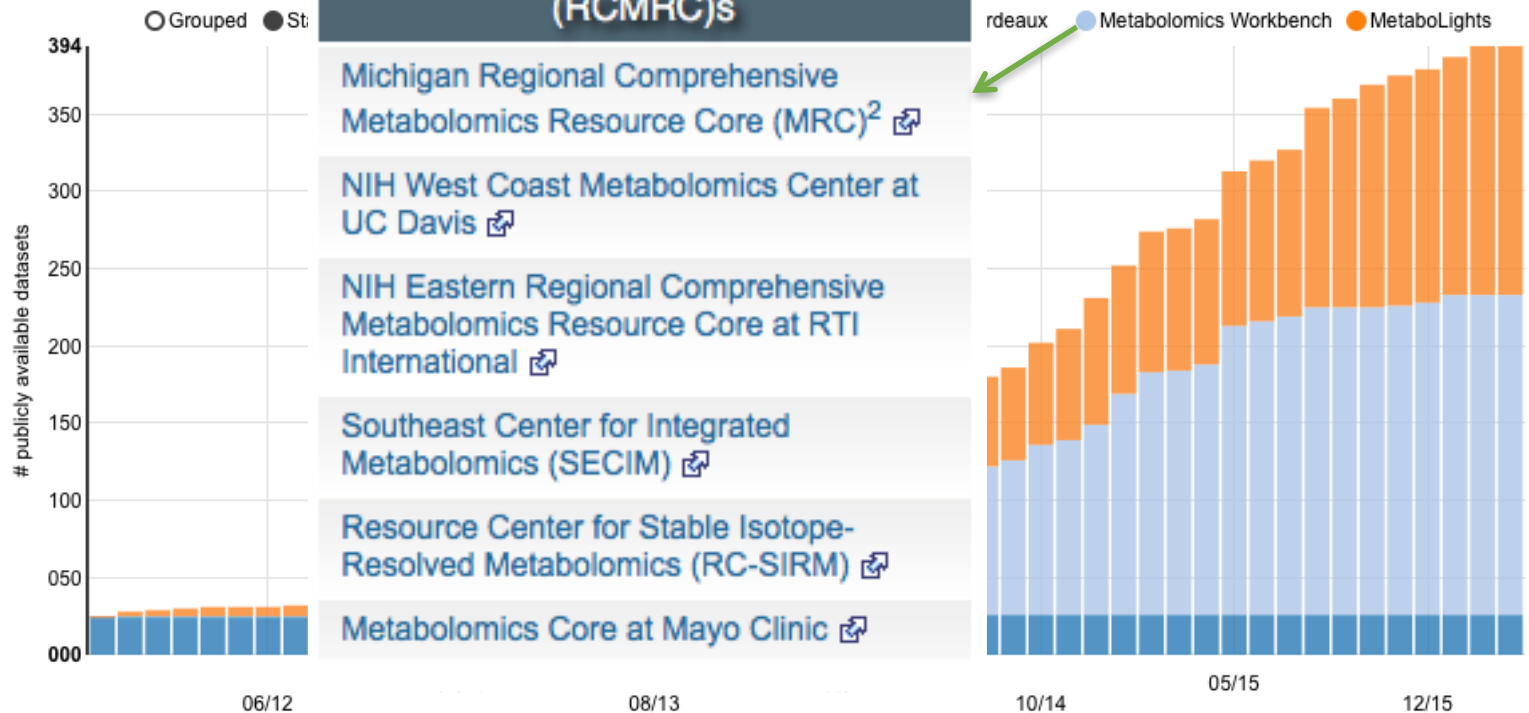


<http://metabolomexchange.org>



# MetabolomeXchange

## Stats



# Use case for metadata: OmicsDI – Collection of omics



## Omics Discovery Index

Home Browse API Databases

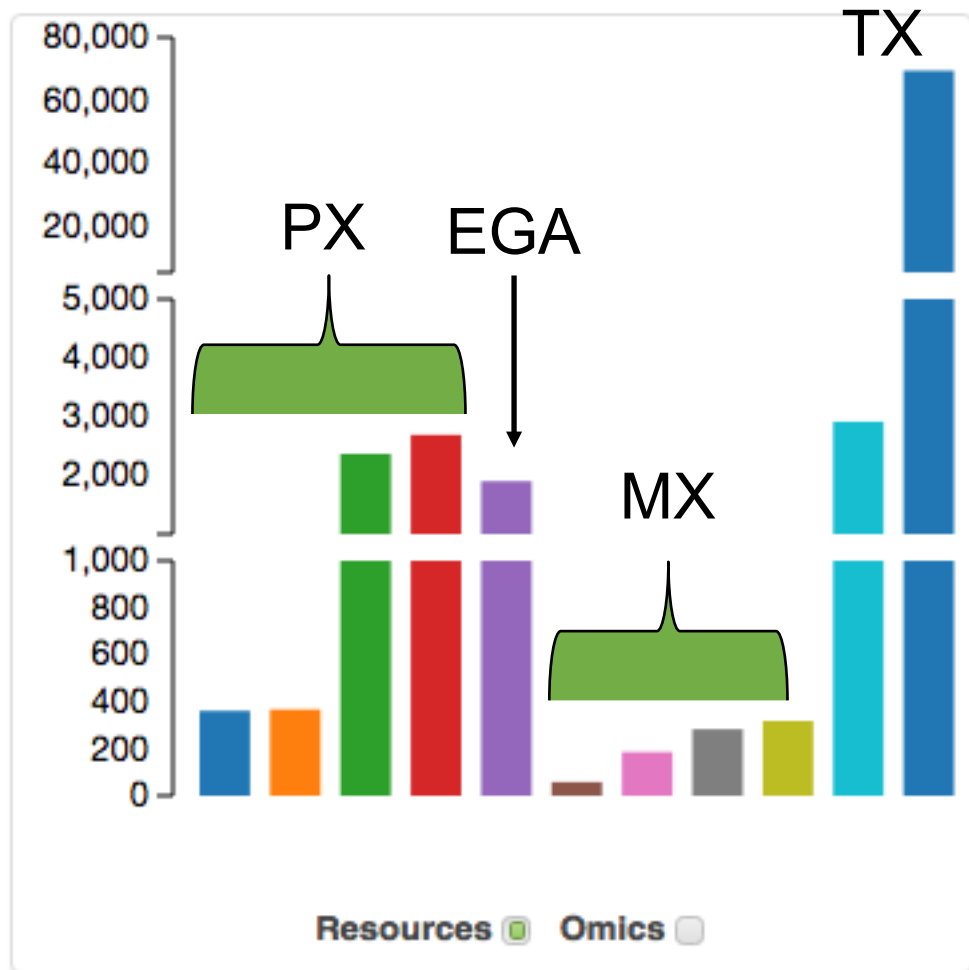
organism, repository, gene, tissue, accession

Examples: cancer, Homo sapiens, Orbitrap, Q9HAU5, Phospho, Hela

revealed further binding  
obtained collected experiments derived  
effects including generated  
following differentially  
**expression** series  
tumor novel transcriptome molecular line  
overall analysis regulation  
factor target sample refer  
**samples** sequencing more  
related patients disease mechanisms  
pathways number  
independent known comparison  
hybridized

Description ☒ Sample ☐ Data ☐

Tissues ☒ Org ☐





\*:\* AND instrument\_platform:"Orbitrap" AND omics\_type:"Metabolomics"

Search

Examples: cancer, Homo sapiens, Orbitrap, Q9HAU5, Phospho, Hela

## Omics Discovery Index

Home Browse API Databases

Help About Feedback

46 Q Results for search term: \*.\* AND instrument\_platform:"Orbitrap" AND omics\_type:"Metabolomics"

Show results for

- P Proteomics (0)
- M Metabolomics (46)
- T Transcriptomics (0)
- G Genomics (0)
- Multi-Omics (0)

Repository

Find your repositories

- ☐ GNPS (14)
- ☐ MetaboLights (22)
- ☐ MetabolomicsWorkbench (10)

Page 1 2 3 4

Page size 15 20

Showing 1 - 15 of 46

Sort by: Accession Relevance Publication date

M Metabolomics-based elucidation of active metabolic pathways in erythrocytes and HSC-derived reticulocytes

Human stem cell derived reticulocytes were compared with mature erythrocytes by metabolomics analysis.  
ORGANISM(S): Homo sapiens

ST000403 | MetabolomicsWorkbench

M TC and B6 untreated plasma in lupus-prone mice lipidomics (part-II)

compare plasma samples from 3 month old lupus-prone (TC) and control (B6) mice  
ORGANISM(S): Mus musculus

ST000310 | MetabolomicsWorkbench

M Untargeted metabolomic analysis of the small intestinal content of malnourished mice

A total of 8 samples from 6 week old, female C57BL/6 mice, treated for 3 weeks with a malnourished diet or a control-fed isocaloric diet.  
Samples were taken from the small intestinal fecal content at the terminus of the ileum.

# Leading to data discovery

[Q Search](#)

Examples: [cancer](#), [Homo sapiens](#), [Orbitrap](#), [Q9HAU5](#), [Phospho](#), [Hela](#)

## Omics Discovery Index

[Home](#) [Browse](#) [API](#) [Databases](#)[Help](#) [About](#) [Feedback](#)

### Dataset Information



#### Metabolomics-based elucidation of active metabolic pathways in erythrocytes and HSC-derived reticulocytes

[Ontology highlight](#)

**ABSTRACT:** Human stem cell derived reticulocytes were compared with mature erythrocytes by metabolomics analysis.

**DATA PROTOCOL:** [HILIC POSITIVE ION MODE](#)

**INSTRUMENT(S):** [Orbitrap](#);

**ORGANISM(S):** [Homo sapiens](#);

**TISSUE(S):** [Blood](#);

[ST000403](#) | [MetabolomicsWorkbench](#)

[JSON](#)[XML](#)

### Similar Datasets

[Hs\\_GSCs](#)

2014-12-31 | [PAe005052](#) | [PeptideAtlas](#)

[Test Metabolomics set](#)

2014-05-02 | [E-TABM-289](#) | [ArrayExpress](#)



[Metabolomic profiling of twenty metabolites from human tissues in six studies](#)

2014-05-02 | [E-TABM-290](#) | [ArrayExpress](#)

[Quantitative Proteomics Reveals](#)

[Metabolic Differences in Homing and Non-Homing Glioma Stem Cell Xenografts and Stromal Cells](#)

2016-02-17 | [PXD001778](#) | [PRIDE](#)

EMBL-EBI



# DATA FORMATS

# Why different formats?



U-Matic (3/4")



VHS



8mm, Hi-8, Digital8



Beta SP



Betamax



VHS-C



MiniDV



DVCam

## COordination of Standards in MetabOlomicS -FP7



# Data Standards, Exchange; What is XML?

- XML stands for E**X**tensible **M**arkup **L**anguage
- XML is a markup language much like HTML
- XML was designed to carry data, not to display data
- XML is designed to be self-descriptive

## NMR analysis

All spectra were recorded on a

<Varian NMR Instrument> Varian VNMRS 600 NMR

Spectrometer </Varian NMR Instrument>

operating at a proton NMR frequency of

<Irradiation frequency>599.83

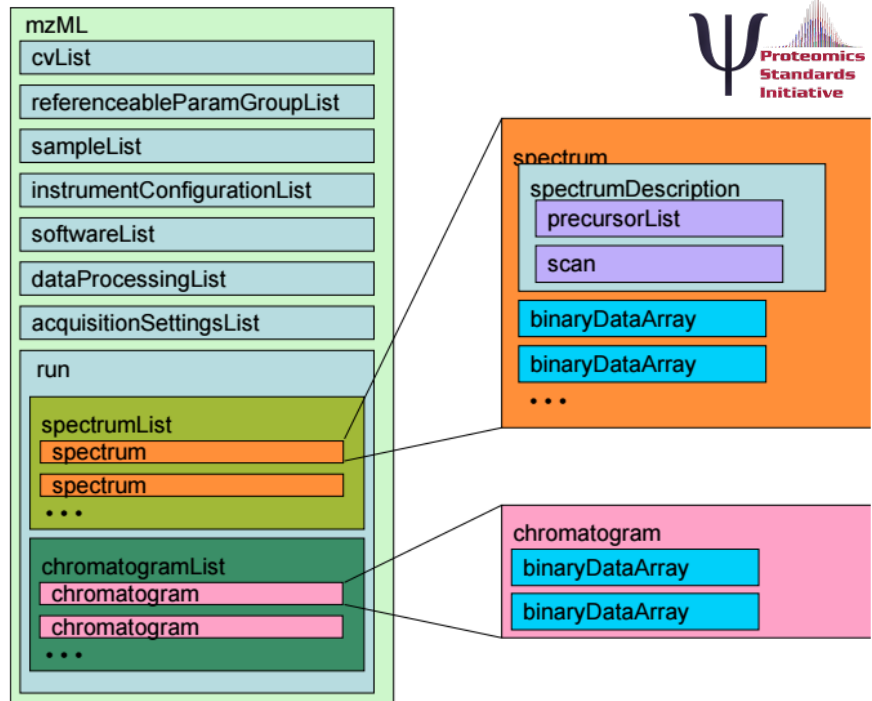
<Megahertz>MHz</Megahertz> </Irradiation frequency>

using a <cryoprobe>5 mm inverse detection

cryoprobe</cryoprobe>.

<acquisition nucleus>1H</acquisition nucleus> NMR

spectra were recorded [...].





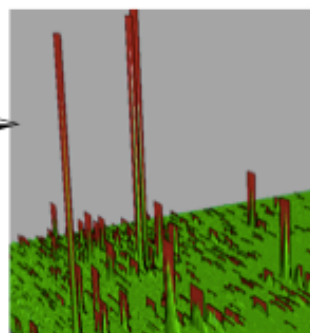
# Data exchange standards in MS

Metadata  
**ISAtab**

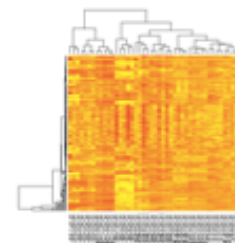
Raw data  
**mzML**

Metabolite  
Identification  
**mzTab**

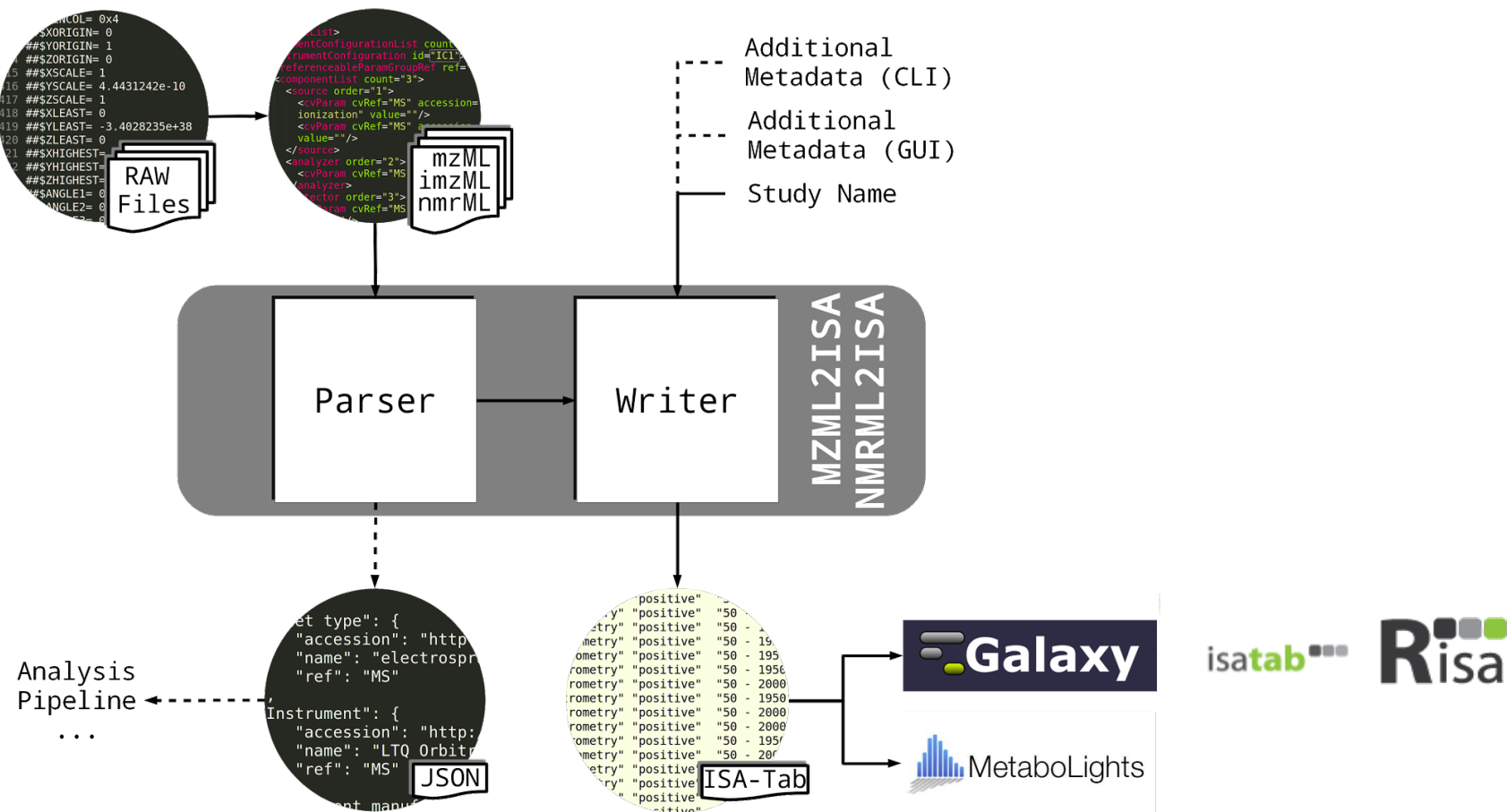
Metabolite  
Quantification  
**mzTab**



	mzmed	rtmed	E25BC1-R1	E25BC1-R2	E25BC1-R3	E25BC4-R1	E25BC4-R2
1	489.67	267.62	96.02	102.01	102.01	102.02	102.01
2	357.96	268.36	254.04	240.03	148.03	238.04	234.04
3	363.09	2072.25	82	95.73	98.36	87.84	85.92
4	212.84	268.04	1944.38	1896.25	1890.21	2068.31	2002.21
5	592.16	1241.43	1046.14	1058.17	1068.18	1002.17	1030.21
6	473.06	1332.09	166.04	168.03	168.02	144.03	158.02
7	155.08	1330.06	712.71	784.22	753.02	729.2	699.6
8	189.2	263.15	143.29	134.7	158.02	143.34	206.02
9	155.06	1566.69	490.49	478.03	451.3	512.93	455.05
10	156.07	1568.47	24.12	78.01	56.16	64.12	29.94
11	486.69	2073.95	24	54.01	4.01	3.99	46.01
12	900.25	1329.76	62.23	60.32	50.2	60.01	61.61
13	603.18	2074.24	20	17.95	8.03	23.95	27.97



# Generating ISA-Tab metadata files from metabolomics XML data



# Tools the way forward!

GitHub, Inc. [US] <https://github.com/ISA-tools/isa-api>

rowling marklin Bookmarks World Time - World TeXMed - Exporting parcel tracking house improvement python and graph slack-channel

## README.md

### ISA API

The open source ISA metadata tracking tools help to manage an increasingly diverse set of life science, environmental and biomedical experiments that employing one or a combination of technologies.

Built around the 'Investigation' (the project context), 'Study' (a unit of research) and 'Assay' (analytical measurement) general-purpose Tabular format, the ISA tools helps you to provide rich description of the experimental metadata (i.e. sample characteristics, technology and measurement types, sample-to-data relationships) so that the resulting data and discoveries are reproducible and reusable.

To find out more about ISA, see [www.isa-tools.org](http://www.isa-tools.org)

To find out who's using ISA and about the ISA development and user community, see [www.isacommons.org](http://www.isacommons.org)

The ISA API aims to provide you, the developer, with a set of tools to help you easily and quickly build your own ISA objects, validate, and convert between serializations of ISA-formatted datasets and other formats/schemas (e.g. SRA schemas). The ISA API is published on PyPI as the `isatools` package.

build passing coverage 63% pypi package 0.1.0

**\*Note that the current version is a very early stage release (v0.1)\***

Authors: The ISA team.

License: This code is licensed under the CPAL License.

Repository: <https://github.com/ISA-tools/isa-api>

ISA team email: <https://groups.google.com/forum/#!forum/isatools>

ISA discussion group: <https://groups.google.com/forum/#!forum/isaforum>

Github issue tracker: <https://github.com/ISA-tools/isa-api/issues>



### MA LIMS

Dashboard Admin Quotes Repository Help

Project: Total fatty acid analysis by GC-QQQ ( Baker IDI)

Project details

Project title: Total fatty acid analysis by GC-QQQ ( Baker IDI)

Description:

Client: 38

Project managers: Komal Kanjia (komal.kanjia@unimelb.edu.au)  
David De Souza (desouzad@unimelb.edu.au)

+ Add - Remove

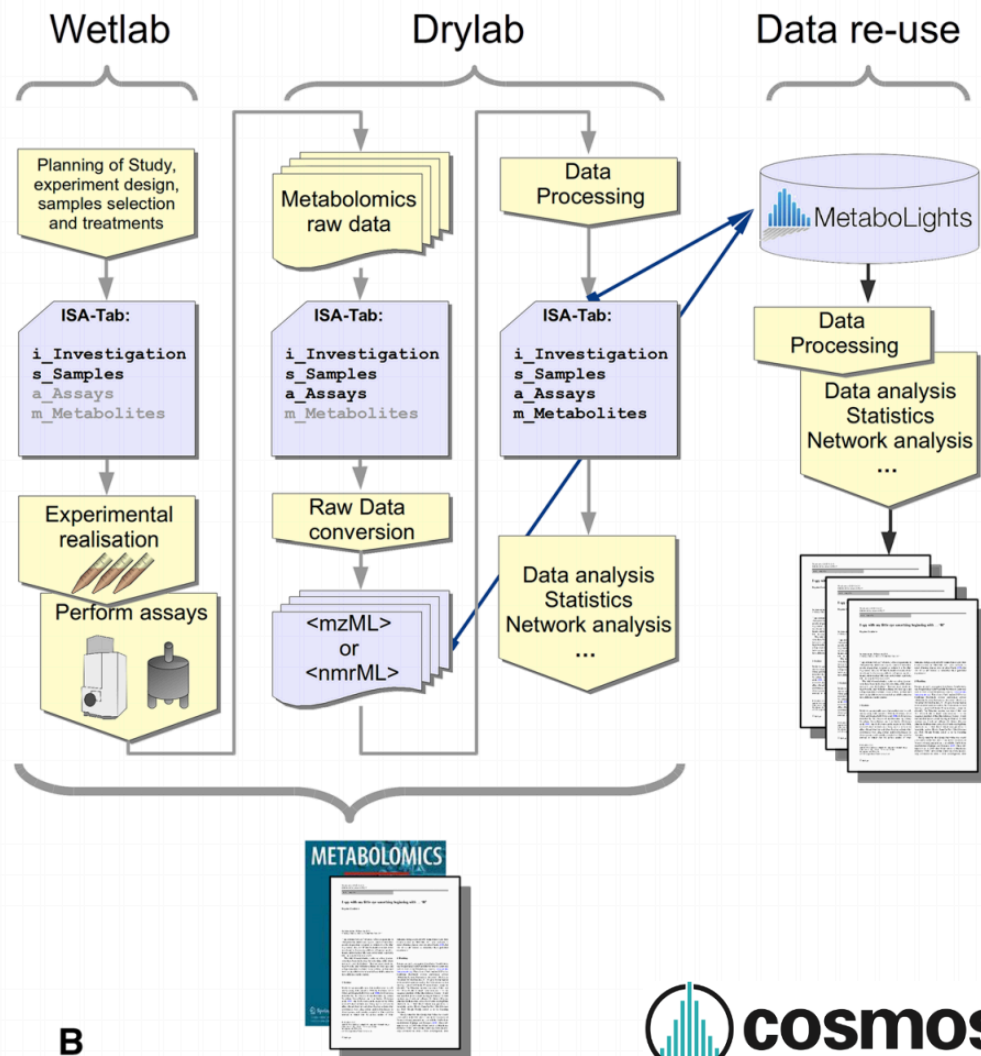
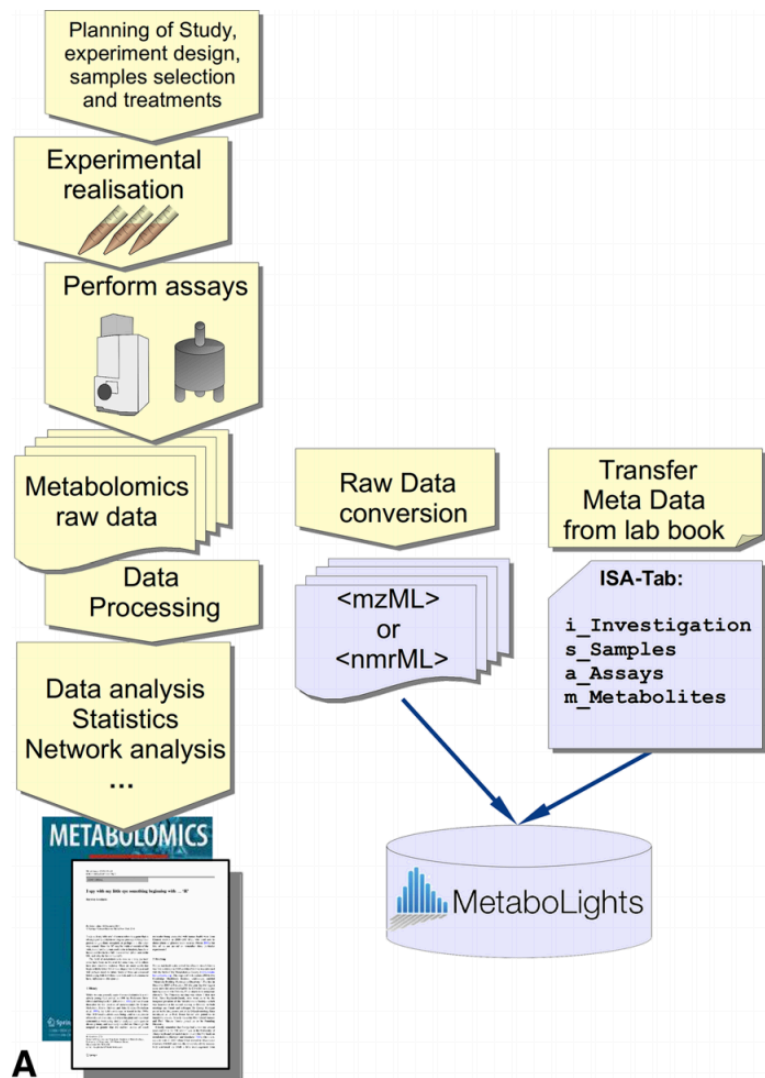
Save ISA-Tab Export

### Missing View Bucket MS/MS Similarity

Sample	Include	Strength
sample_1.d	<input checked="" type="checkbox"/>	3
sample_2.d	<input checked="" type="checkbox"/>	3
sample_3.d	<input checked="" type="checkbox"/>	3
sample_4.d	<input checked="" type="checkbox"/>	3
sample_5.d	<input checked="" type="checkbox"/>	3
sample_6.d	<input checked="" type="checkbox"/>	3
Coffee_strength_9_Sample_1.d	<input checked="" type="checkbox"/>	9
Coffee_strength_9_Sample_2.d	<input checked="" type="checkbox"/>	9
Coffee_strength_9_Sample_3.d	<input checked="" type="checkbox"/>	9
Coffee_strength_9_Sample_4.d	<input checked="" type="checkbox"/>	9
Coffee_strength_9_Sample_5.d	<input checked="" type="checkbox"/>	9
Coffee_strength_9_Sample_6.d	<input checked="" type="checkbox"/>	9

Toggle Include State  
Import attributes  
Export as ISA-TAB

# Current way and ideal



# DATA ANALYSIS

## THE MISSING LINK

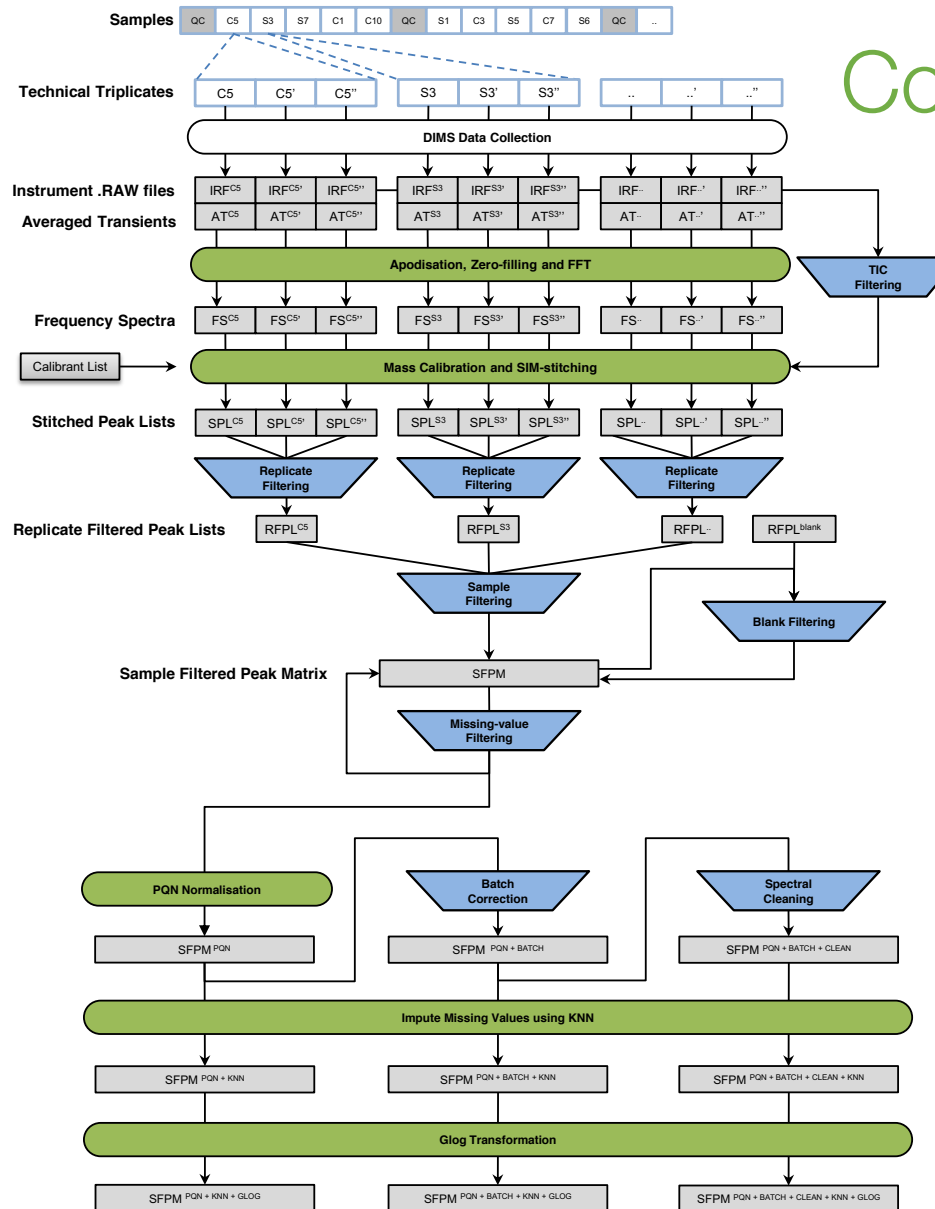


# What software we have –which one should I choose?

Type of Tool	Number
LC/MS	93
GC/MS	32
NMR	24
Metabolite Identification	29
Lipid Identification	6
Lipidomics - Other	2
Statistical Analysis	13
Pathway Analysis	9
Total	208

Rachel Spicer

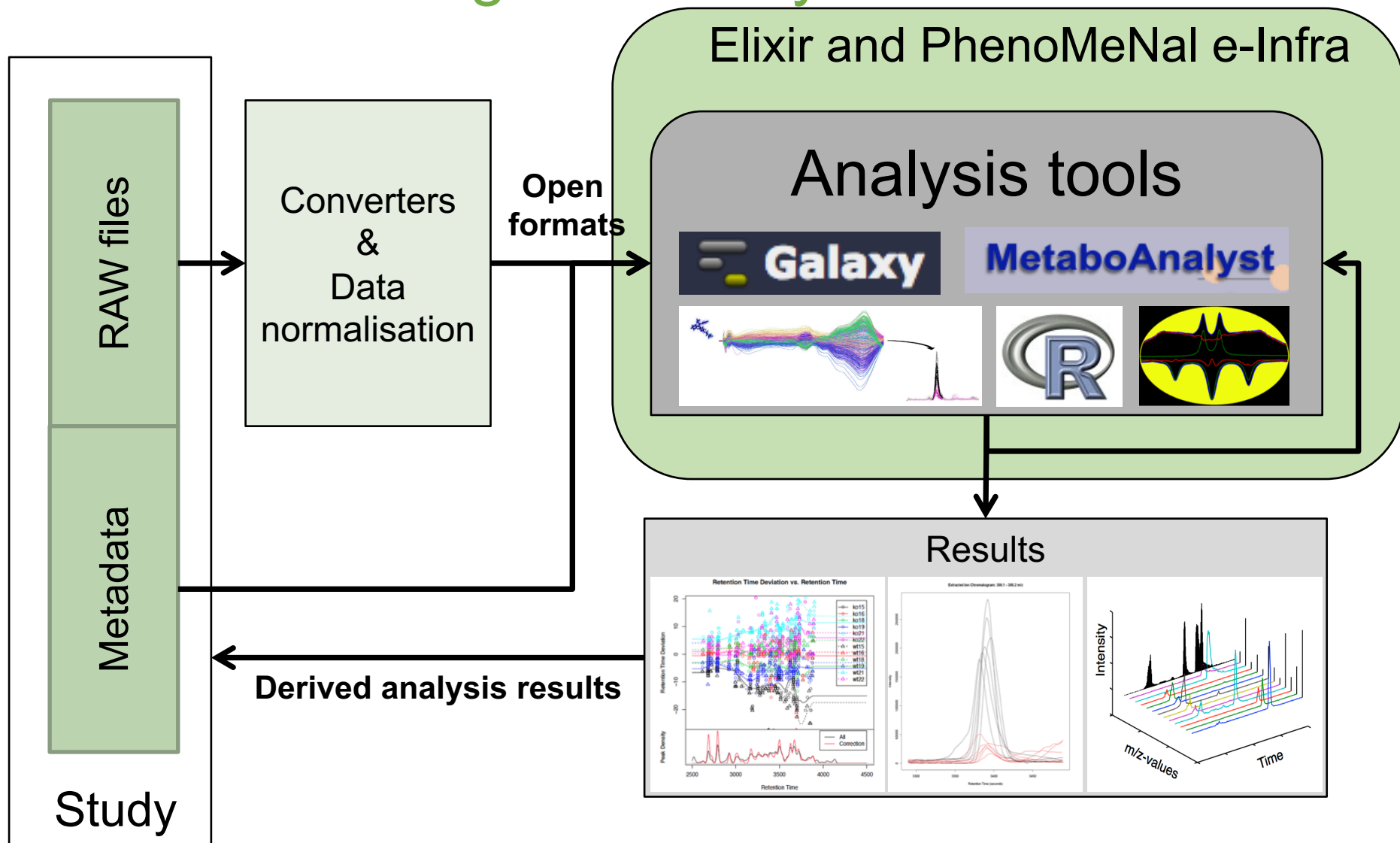
# Complex analysis pipelines



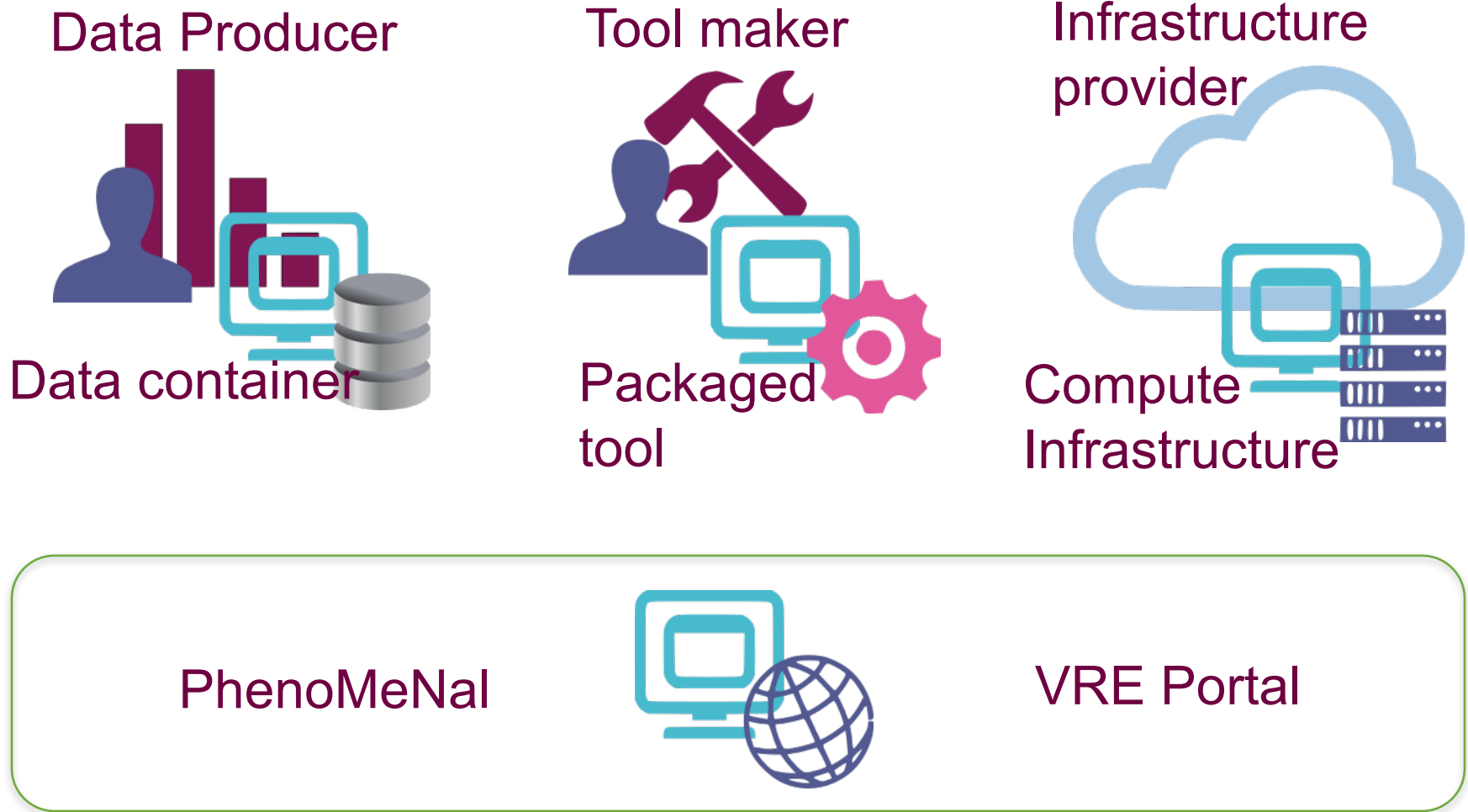
The image shows the MetaboLights website interface for the MTBLS79 dataset. The header includes the MetaboLights logo and a search bar. The main content area displays the dataset title: "MTBLS79: Direct infusion mass spectrometry metabolomics dataset: a benchmark for data processing and quality control". Below the title, there are links for "Share Study" and "View all files". The submission information is shown: "Submitted: 01-Apr-2014, Release date: 05-Jun-2014" and "Other identifiers: SDN\_DIMS". The dataset is categorized under "Study Design Description", "Protocols", "Assay", and "Study Files". At the bottom, there are links for "Download whole study", "Download metadata" (highlighted with a red box), and "View all files".



# MetaboLights – Analysis workflow

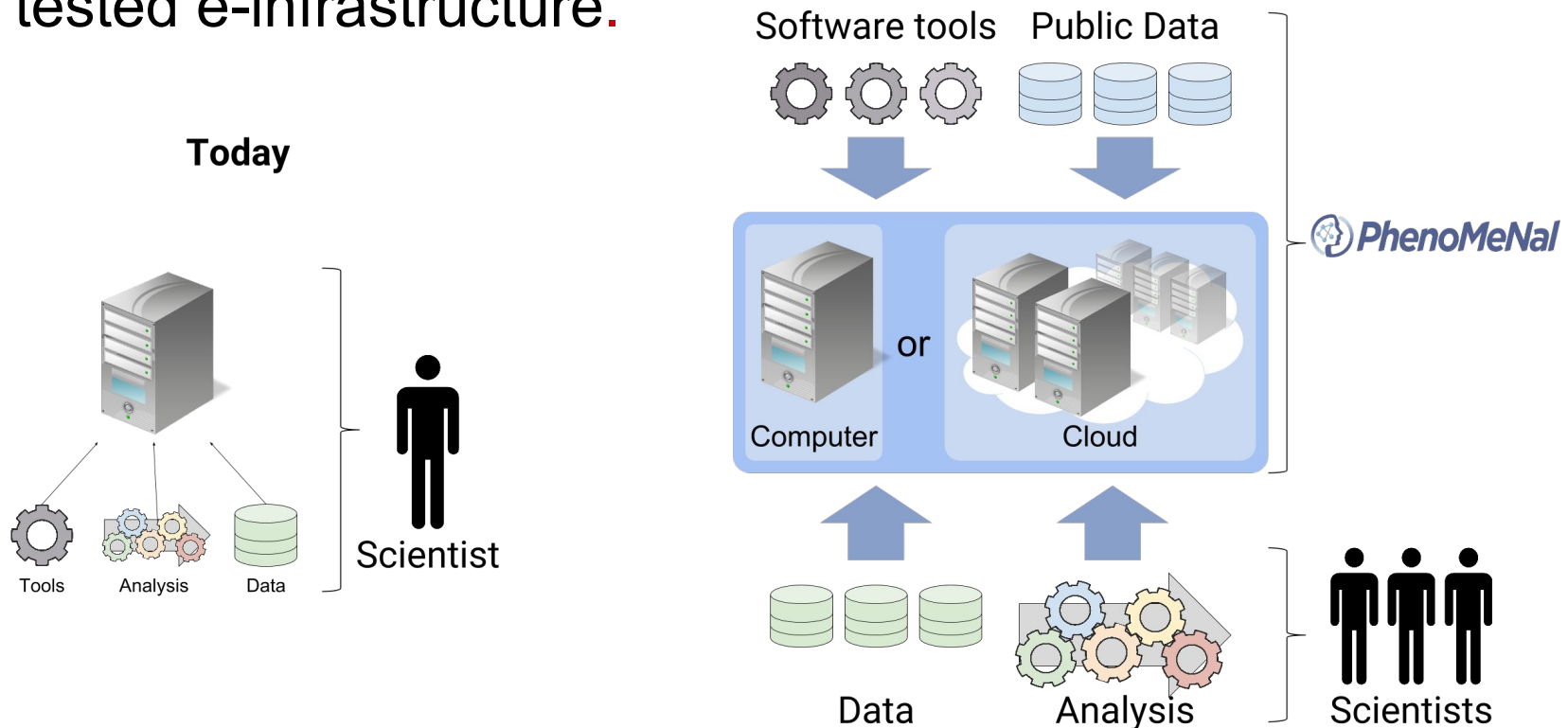


# PhenoMeNal - Goal



# Key objectives

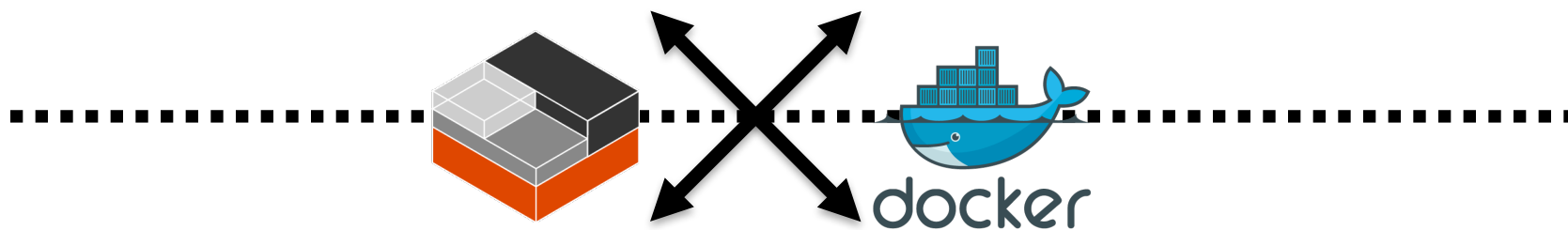
- Understand the computational needs of the Metabolomics Community.
- Integrate and scale existing Open Source tools into a well-tested e-infrastructure.



# Major revolution



# Same in software



Developer's



PI's



Cluster



Cloud



Collaborator's

# VRE Portal

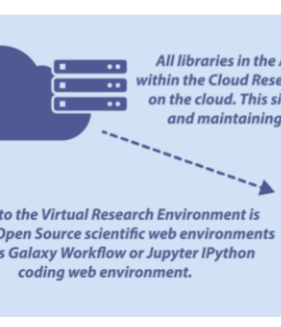
- Three usability rounds
- 80% functionality running.
- Public instance access.
- App Library, hooked to EGI AppDB.
- Documentation.

<http://portal.phenomenal-h2020.eu/>

**PhenoMeNaL Gateway** Cloud Research Environment Portal

[Home](#)    [Cloud Research Environment](#)    [App Library](#)    [Help](#)

---



All libraries in the App Library run within the Cloud Research Environment on the cloud. This simplifies running and maintaining applications.

Access to the Virtual Research Environment is through Open Source scientific web environments such as Galaxy Workflow or Jupyter IPython coding web environment.

## An easy to use, cloud based scalable software infrastructure for metabolomic research

Want to give it a go?

Create  
Cloud Research Environment

Find out more

Test drive our Cloud Research Environment

Galaxy Workflow

or

Jupyter IPython

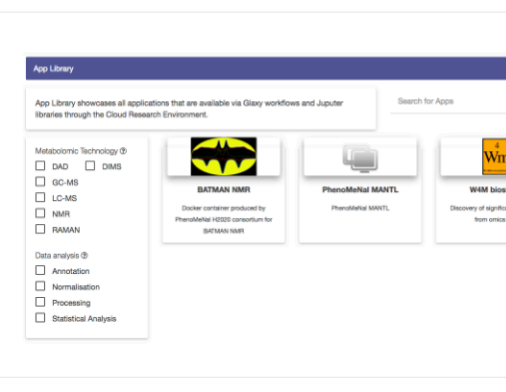
Note that this is a public instance accessible by everyone

---

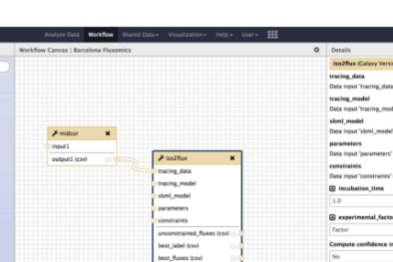
## The open-source App Library provides a catalogue of free Metabolomic data analysis libraries available within the Cloud Research Environment

With user feedback and ratings it is easier to choose the best software for your analysis

Browse App Library



---

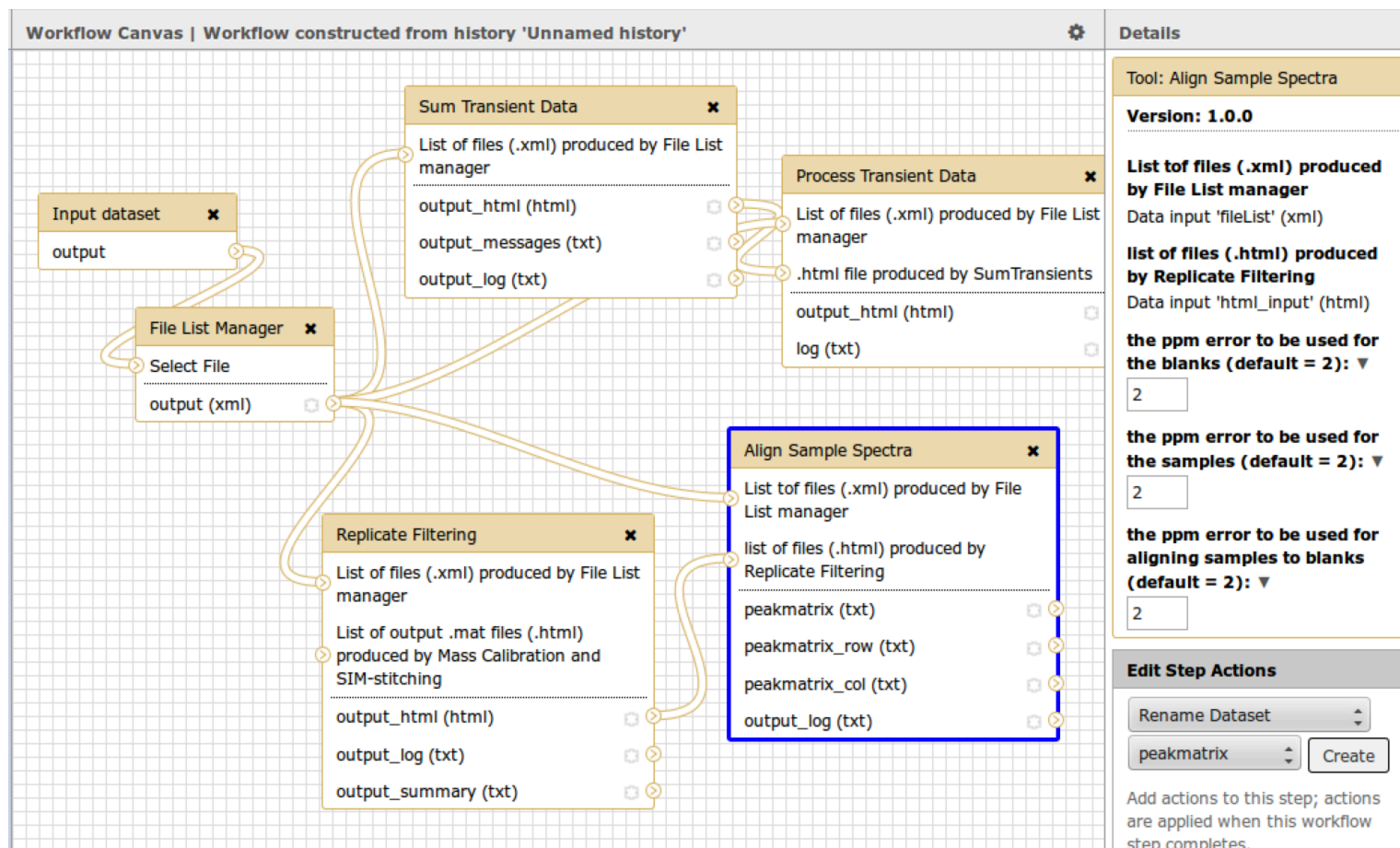


## Access your Cloud Research Environment through standard scientific open-source web environments, Galaxy Workflow tool and Jupyter coding environment



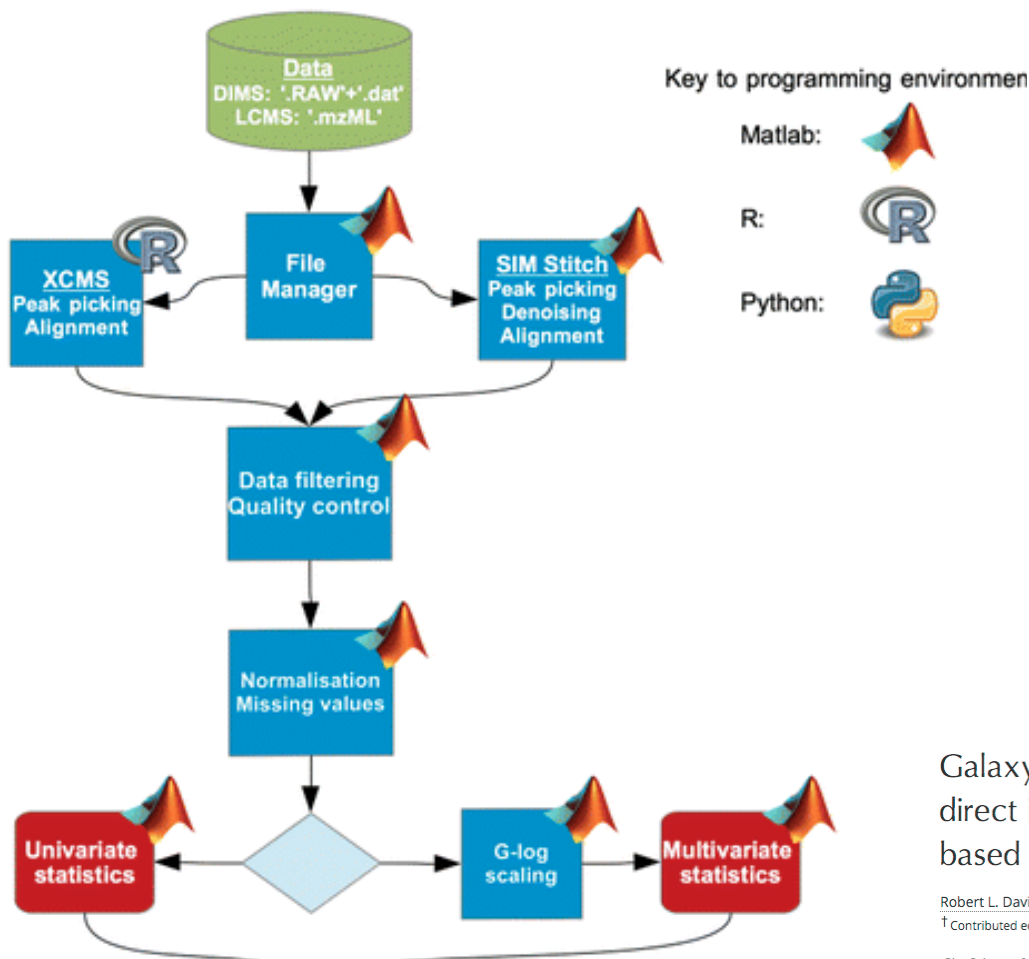
# Why workflow?

View, share, edit, rerun workflow





# Birmingham galaxy-m metabolomics workflow



- Many tools
- Many languages
- Complex to learn
- Many parameters
- Complex to report

Galaxy-M: a Galaxy workflow for processing and analyzing direct infusion and liquid chromatography mass spectrometry-based metabolomics data

Robert L. Davidson<sup>†</sup>, Ralf J. M. Weber<sup>†</sup>, Haoyu Liu, Archana Sharma-Oates and Mark R. Viant

<sup>†</sup> Contributed equally

*GigaScience* 2016 5:10 | DOI: 10.1186/s13742-016-0115-8 | © Davidson et al. 2016

Received: 5 March 2015 | Accepted: 6 February 2016 | Published: 23 February 2016

Open Peer Review reports



UNIVERSITY OF  
BIRMINGHAM

(GIGA)<sup>m</sup>  
SCIENCE

华大基因  
BGI

NERC  
SCIENCE OF THE  
ENVIRONMENT

**Galaxy / 4 / Metabolomics**

Tools 

search tools

**Upload File** from your computer

### Export Data

LC-MS

## Format Conversion

## Preprocessing

### Normalisation

## Quality Control

### Statistical Analysis

### Annotation

GC-MS

## Preprocessing

## Normalisation

## Quality Control

### Statistical Analysis

### Annotation

## NMR

## Preprocessing

## Normalisation

## Quality Control

### Statistical Analysis

### Annotation

## COMMON TOOLS

## Data Handling

## Text Manipulation

### Filter and Sort

### Join, Subtract and Group

## Statistics

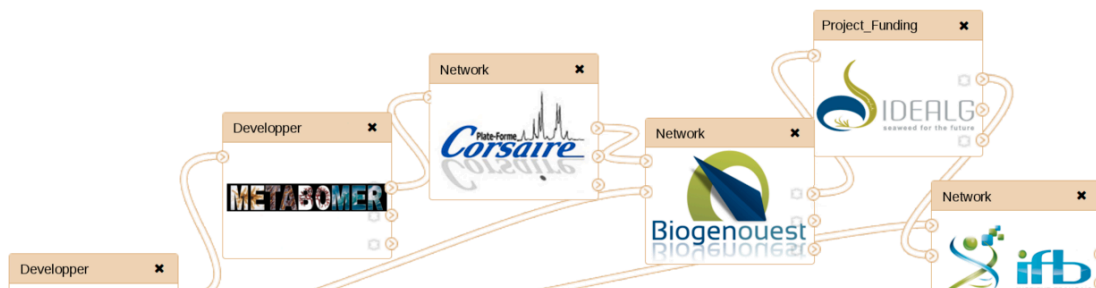
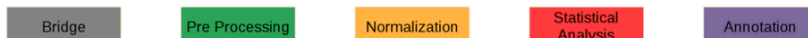
### Graph/Display Data

## Deprecated Tools

## Multiple regression

## Workflows

- All workflows



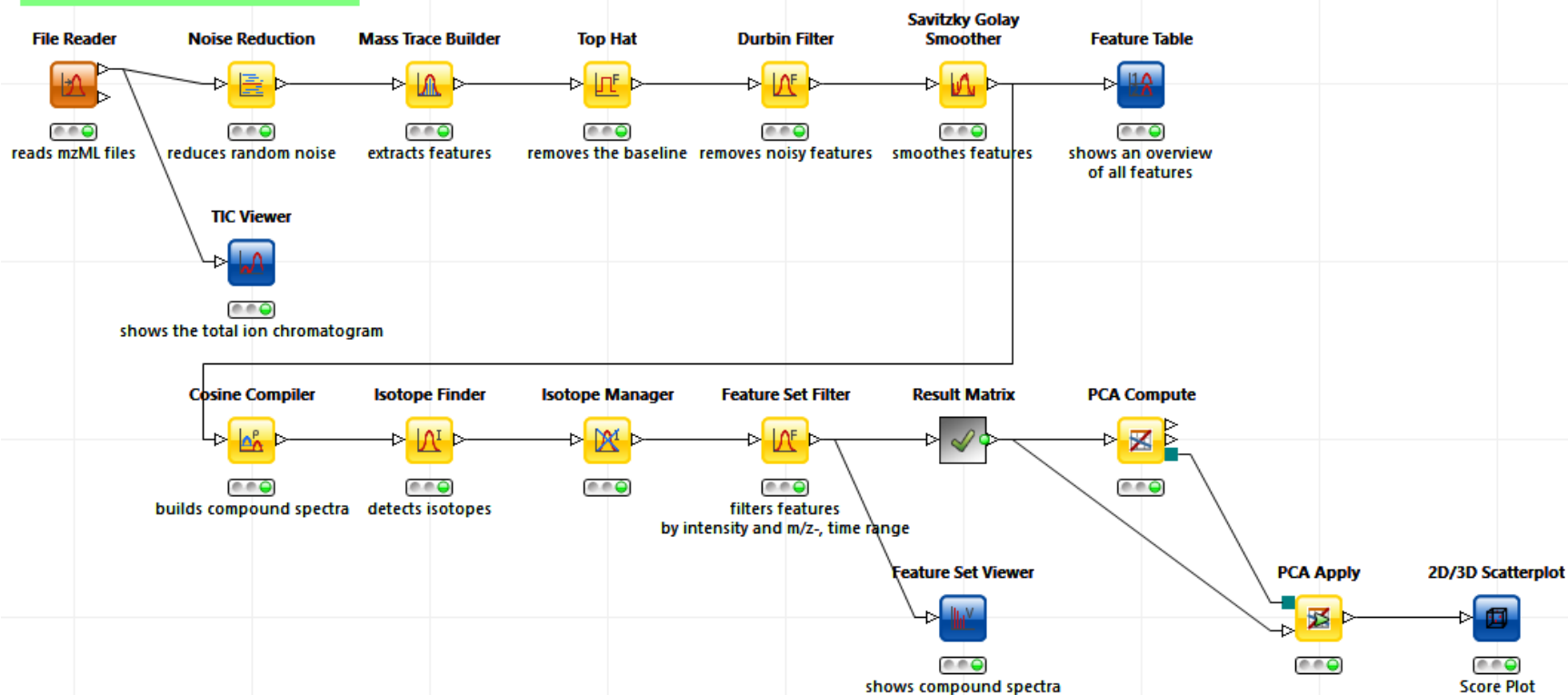
# MassCascade EMBL-EBI

## MassCascade, Tomato samples

LC-MS positive ion mode

mzML:

- 3 pooled samples
- 3 WT QC samples



<https://bitbucket.org/sbeisken/masscascadeKNIME/wiki/ExampleWorkflows>

# MetaboLights – The team



Kenneth Haug



Reza Salek



Kalai Jayaseelan



Mark Williams



Venkata  
Chandrasekhar



Keeva Cochrane



Jose Ramon Macias  
Gonzalez



Xuefei Li (MRC)



Christoph Steinbeck



Jules Griffin (UC/MRC)

Previous: Paula de Matos, Mark Rijnbeek, Tejasvi Mahendraker, Pablo Conesa

# EBI PhenoMeNal – The team



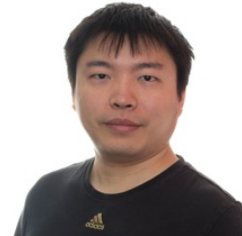
Kenneth Haug



Reza Salek



Pablo Moreno



Sijin He



Christoph Steinbeck



Namrata Kale



# COSMOS consortium





# PhenoMeNal consortium



# Funding and Collaborators



Improving health through nutrition research

