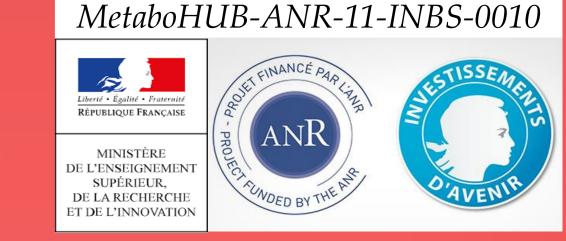


MetaboHUB: a national infrastructure for metabolomics and fluxomics (<u>http://www.metabohub.fr</u>)



MetaboHUB: Innovation, development and training dedicated to metabolomics and fluxomics

<u>Camille Bénard</u>, Cecilia Berges, Thierry Berton, Raphael Bir, Noémie Butin, Salimata Diarrassouba, Sylvain Emery, Maria Fatarova, Maud Heuillet, Ulli Hohenester, Hanna Kulyk-Barbier, Sylvain Kenan, Nadia Lamari, Marie Lefebvre, Maria-Helena Meireles, Nils Paulhe, Laura Prouteau, Fabien Riols, Léa Roch, Simon Roques, Pierrick Roger-Mele, Khoury Spiro, Samuel Terrier, Laetitia Theron, Fanny Viard, Vanessa Zhendre, Jean-Emmanuel Sarry, Christophe Caron, Caroline Sautot, Christophe Junot, Dominique Rolin and **all other MetaboHUB consortium members**

Metabolomics and fluxomics require several complementary analytical and computational approaches such as nuclear magnetic resonance (NMR), mass spectrometry (MS) and bioinformatics.

To meet the metabolomics community needs involving large-scale programs, MetaboHUB is developing :

- Robotic workflows enabling high-throughput cell culture and sample preparation
- Analytical procedures for metabolic profiling, and methods for absolute quantitation

Many training sessions and workshops are organized on these technologies: http://www.metabohub.fr/next-trainings.html

Bioinformatics resources are of prime importance for analyzing and handling the large amount of data generated in such studies:

- A web portal "MAMA" gives the entire community access to these developments and facilities
- Three long-term sustained e-MetaboHUB platforms offer online data processing, analysis, and interpretation

MAMA MetaboHUB Analyst MAnager

- Analytical request centralisation and management for MetaboHUB users
- Create your account and enter your analytical request
- mama-webapp.metabohub.fr

etExplore

In silico global analysis of metabolism

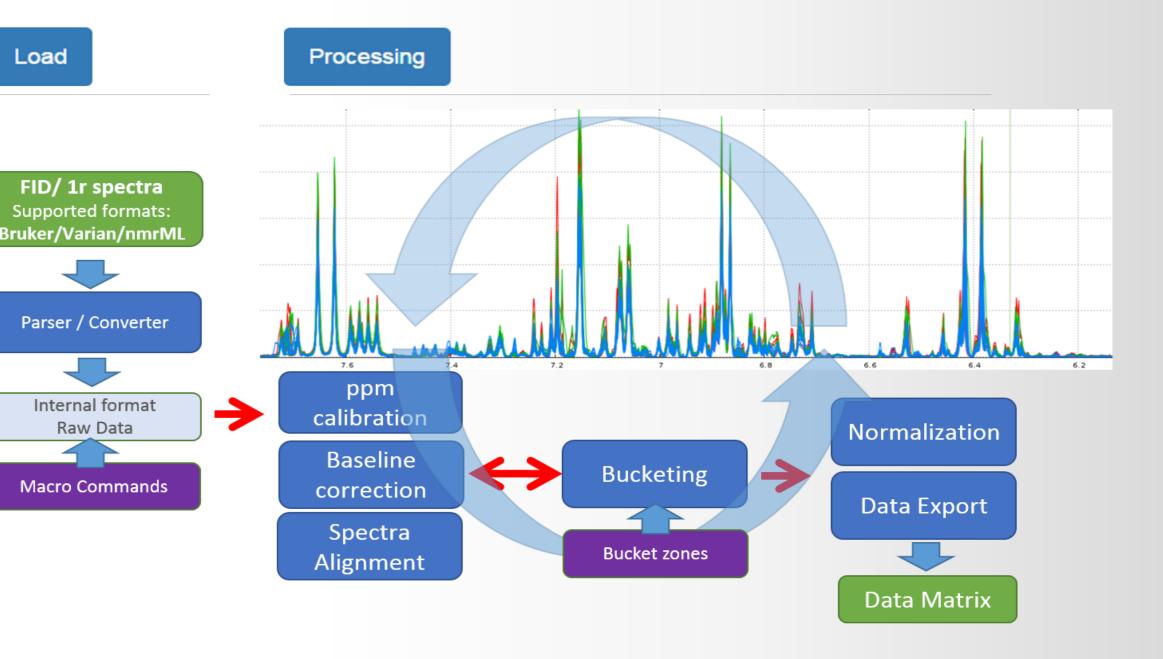
Import/export networks
Chemical library mapping



A complete set of tools for processing and visualization of 1D NMR data

nformation type

- Interactive interface based on spectra visualization
- Open-source software
- > 800 users from 5 continents, 3,100 sessions
 - since July 2016
- mrprocflow.org



Supplementary Importing files

(optional)

- Collaborative curation
- Pathway enrichment
- Omics data mapping
- Flux computations
- Network visualization
- www.metexplore.fr



0 € to use it, 10 developers, >300 persons trained, >400 registered users, >1,000 networks

Wm Workflow4metabolomics

- > 40 modules for data processing, statistical analysis, and annotation
- LC-MS, FIA-MS, GC-MS, and NMR
- Galaxy environment
- Referencing of workflows (DOI)
- > 800 users

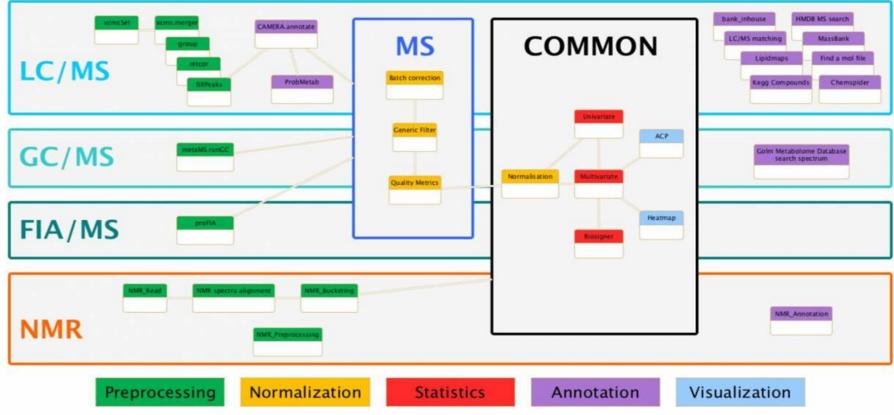
xkflow4metabolomi

- Trainings with tutoring on your own data
- In partnership with the French Institute of Bioinformatics (IFB)
- workflow4metabolomics.org



Module

processing



Examples of two proofs of concept projects designed to apply the MetaboHUB high-value service in health and disease fields:

An investigation of the links between nutrition and chronic metabolic diseases within the Canadian NuAge cohort :



Lipidomic and metabolomic phenotyping

Statistical methods for longitudinal studies and data integration

Metadata and data management, data analysis workflows

Metabolomic and fluxomic studies on acute myeloid leukemia to highlight new therapeutic targets and strategies:

- Quantitative metabolomics by LC-MS/MS of acute myeloid leukemia (AML) cells
- Reconstitution of metabolic fluxes in AML cells
- Integrative omics and in silico modelling

MetaboHUB is also involved in: 019-021-035-043-045-055 P2-P12-P22-P24-P43-P47-P55-P73-P79-P82-P108-P129-P146-P147-P151-P154-P170-P181-P184-P188-P192-P226-P231-P239-P244



References

Boutzen *et al., J Exp Med.*, 2016, 213: 483-497. Cottret *et al., Nucleic Acids Res.,* 2010, 38: W132-7. Farge *et al., Cancer Discov.*, 2017, 7: 713-735. Giacomoni *et al., BioInformatics*, 2015, 31: 1493-1495. Guitton *et al., Int J Biochem Biol.*, 2017. Jacob *et al., Metabolomics*, 2017, 13: 36.

SMMAP 2017 Paris, France 2-5 October 2017

