



HAL
open science

Technological developments and opportunities with Workflow4Metabolomics

Mélanie Pétéra, Cécile Canlet, Romain Dallet, Yann Guitton, Gildas Le Corguillé, Jean-Francois Martin, Stéphanie Monnerie, Estelle Pujos-Guillot, Julien Saint-Vanne, Marie Tremblay-Franco, et al.

► To cite this version:

Mélanie Pétéra, Cécile Canlet, Romain Dallet, Yann Guitton, Gildas Le Corguillé, et al.. Technological developments and opportunities with Workflow4Metabolomics. European RFMF Metabomeeting 2020, Jan 2020, Toulouse, France. , 262 p., 2020, Oral and Poster Abstracts European RMF Metabomeeting 2020. hal-02497719

HAL Id: hal-02497719

<https://hal.science/hal-02497719>

Submitted on 3 Mar 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution - NonCommercial - NoDerivatives 4.0 International License

Technological developments and opportunities with Workflow4Metabolomics



Mélanie PÉTÉRA¹; Cécile CANLET^{4,5}; Romain DALLET³; Christophe DUPÉRIER¹; Yann GUITTON²; Gildas LE CORGUILLÉ³; Jean-François MARTIN^{4,5}; Stéphanie MONNERIE¹; Estelle PUJOS-GUILLOT¹; Julien SAINT-VANNE²; Marie TREMBLAY-FRANCO^{4,5}; W4M Core Team; Franck GIACOMONI¹



¹ Université Clermont Auvergne, INRAE, UNH, Plateforme d'Exploration du Métabolisme, MetaboHUB Clermont, F-63000 Clermont-Ferrand, France

² Laboratoire d'Étude des Résidus et Contaminants dans les Aliments (LABERCA), Oniris, INRAE, UMR 1329, 44307, Nantes, France

³ ABiMS, FR2424 CNRS-UPMC, Station Biologique, Place Georges Teissier, 29680, Roscoff, France

⁴ Toxalim – Research Center in Food Toxicology, Toulouse University, INRAE UMR 1331, ENVT, INP-Purpan, Paul Sabatier University, F-31027 Toulouse, France

⁵ Metatoul-AXIOM platform, National Infrastructure for Metabolomics and Fluxomics, MetaboHUB, Toxalim, INRAE UMR 1331, F-31027 Toulouse, France



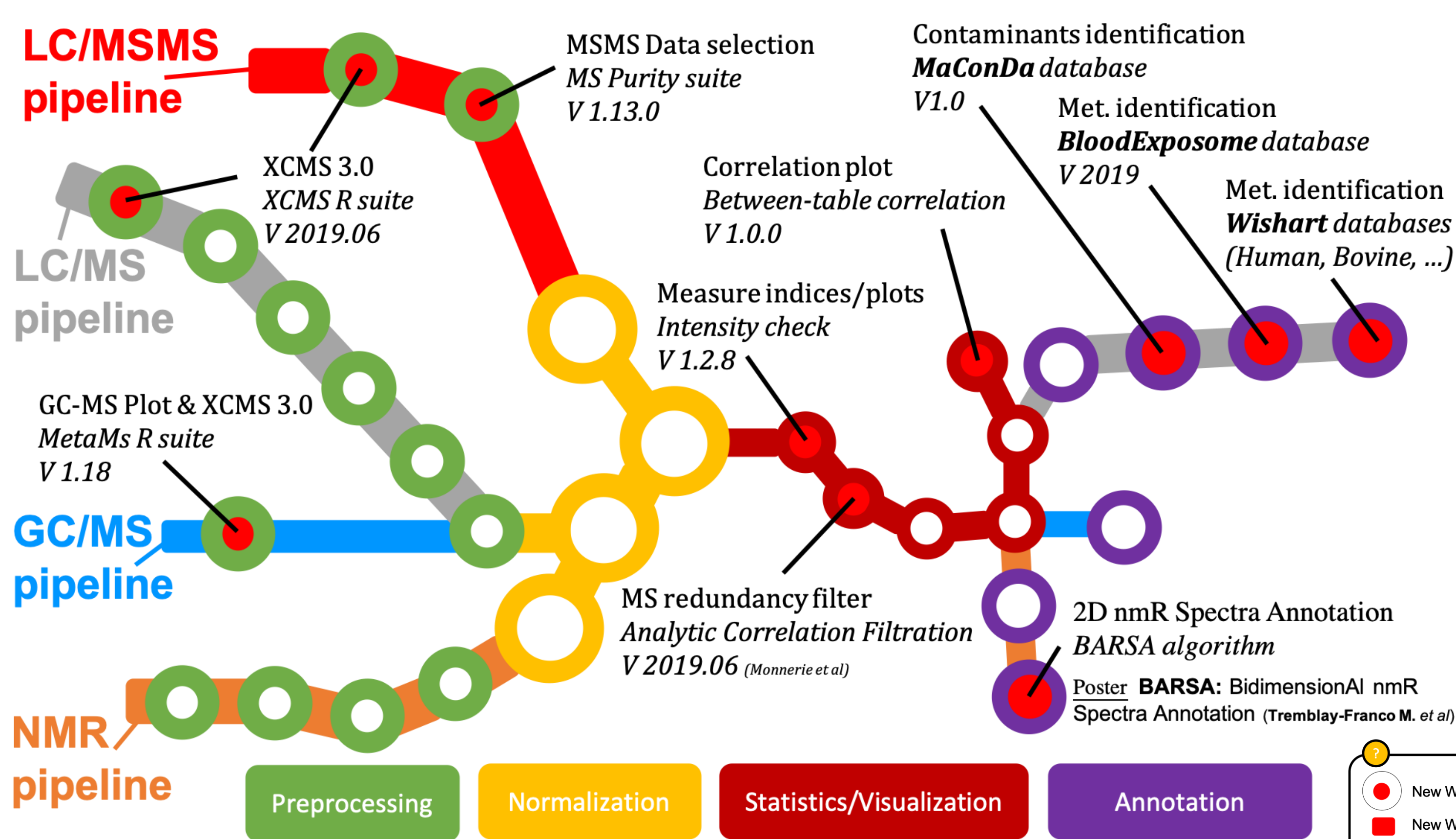
Introduction

Metabolomics data analysis is a complex, multistep process, constantly evolving with the development of new analytical technologies, mathematical methods, bioinformatics tools and databases. **Workflow4Metabolomics** is a collaborative portal dedicated to metabolomics data processing, analysis and annotation for the Metabolomics community. In the **3.0 version**, the W4M core team proposes new upgrades for LC-MS, GC-MS and NMR pipelines, including new preprocessing, quality control, statistical analysis and annotation tools. W4M aims to promote open science in Metabolomics and facilitate knowledge dissemination by providing new community resources.

New W4M LC-MS, LC-MSMS, GC-MS and NMR pipelines

The W4M core team makes continuous upgrades including pipeline enhancement, tool updates and new component development. The V3.0 of the W4M infrastructure integrates:

- A new pipeline, LC-MSMS data specific, including *MS Purity*^[1]
- A major upgrade of the data extraction tools' suite with *XCMS 3.0*^[2]
- Data filtering and visualization steps based on *Analytic Correlation Filtration*^[3] and *Between-table correlation* tools.
- New database resources for metabolite and contaminant annotation^[4,5,6] and the BARSAs new algorithm for NMR-2D spectral annotation.



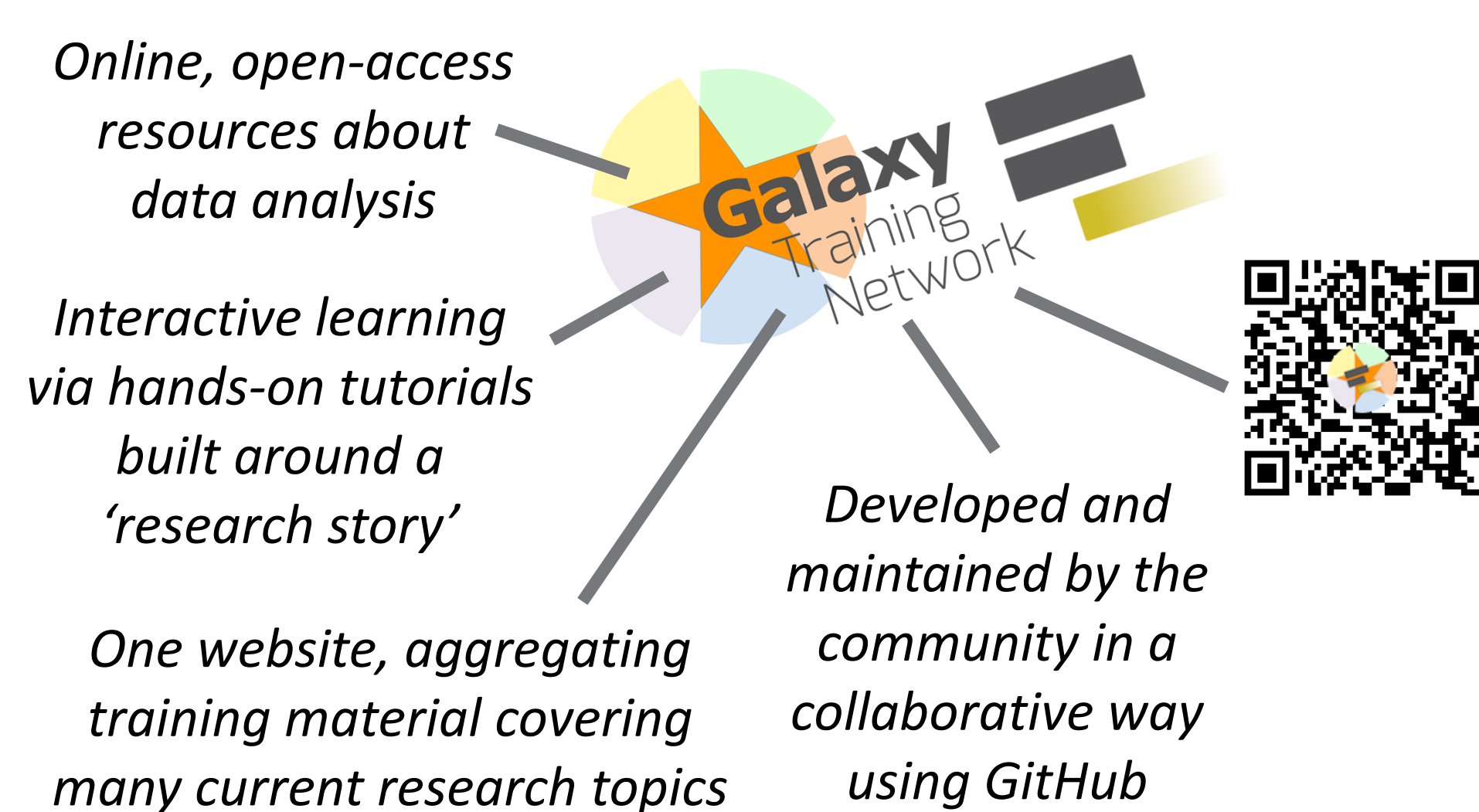
W4M NEWS
BREAKING

The **W4M** infrastructure will join the **usegalaxy.fr** initiative in 2020! More computational power resources, more data storage and more tools and data dynamic visualization – Watch this space!

Open Science and open training materials

W4M is fully involved in the Open science movement. After providing Digital Object Identifiers (DOI) for user data history references^[7], new actions include producing training materials based on the Galaxy Training Network (GTN) concept and format.

What is the GTN?



What are W4M GTN contributions?

- Galaxy / Workflow4Metabolomics
- Get to grips with metabolomics data analysis at your own pace using new Galaxy Training Materials provided by W4M!
- Galaxy Training! Introduction to Metabolomics
 - Galaxy Training! Mass spectrometry: LC-MS analysis
 - Galaxy Training! Mass spectrometry: LC-MS preprocessing advanced (coming soon)
 - Galaxy Training! Mass spectrometry: MSMS analysis with msPurity package (coming soon)

Gathering "open source" contributions

W4M contributes to and promotes the use of metabolomics software and open-source software package production. Contributors share new metabolomics data analysis tools compliant with the galaxy framework on the new GitHub **"tools-metabolomics"** repository. This public repository aims to provide:



- A Galaxy wrapper code review based on IUC (Galaxy Intergalactic Utilities Commission) standards and best practices
- MyTool showcase on galaxy.workflow4metabolomics.org and on usegalaxy.eu
- Tools annotation following bio.tools registry guidelines (coming soon)

Join us on workflow4metabolomics.org!

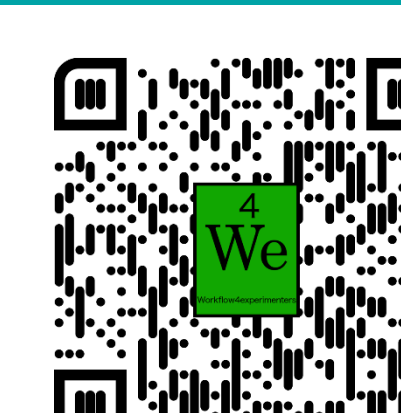
W4M web portal:



W4M pipelines:



W4E 2020 course:



Funding:

La Région
Auvergne-Rhône-Alpes

