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Technological developments and opportunities with Workflow4Metabolomics



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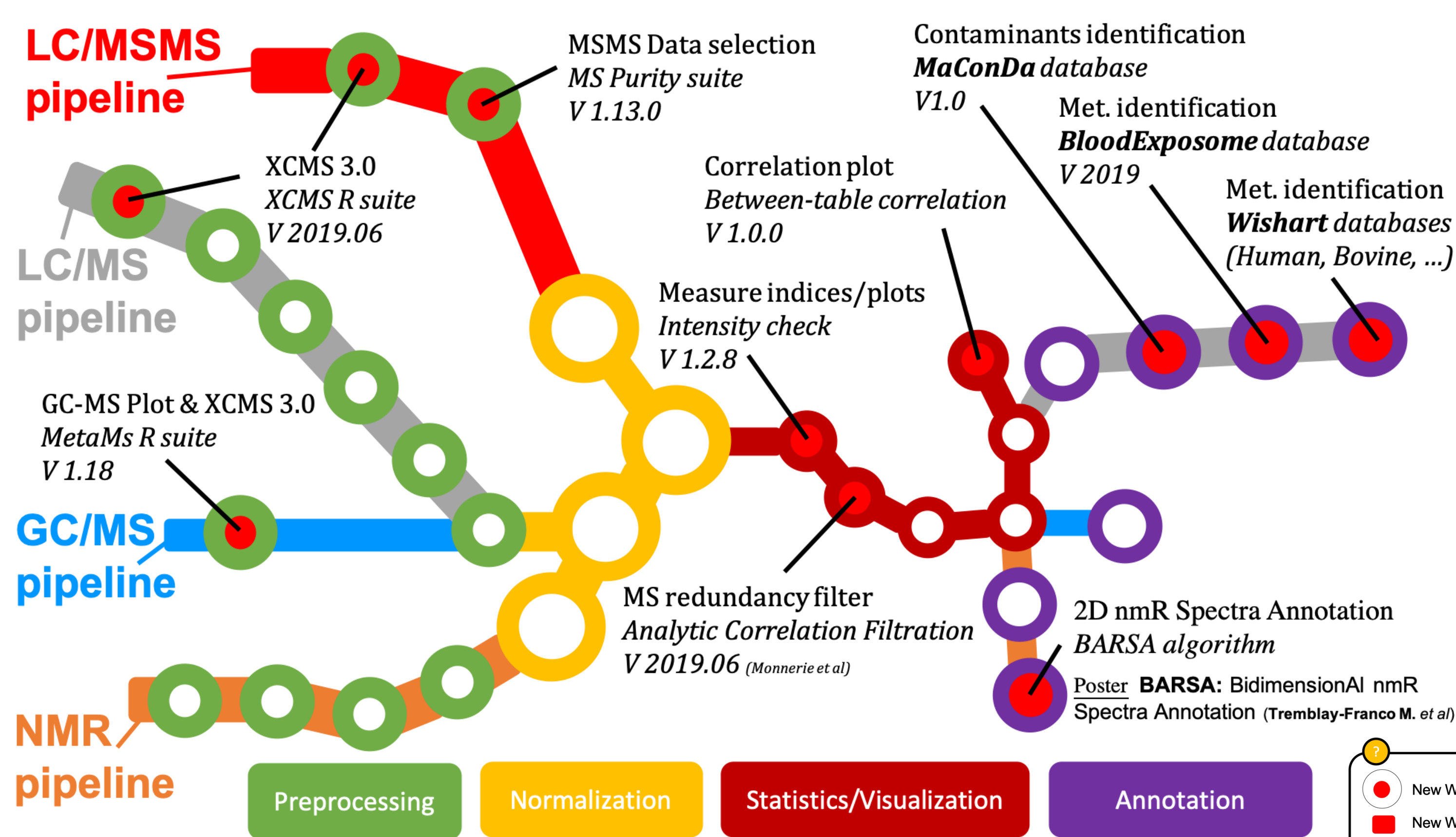
Introduction

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.

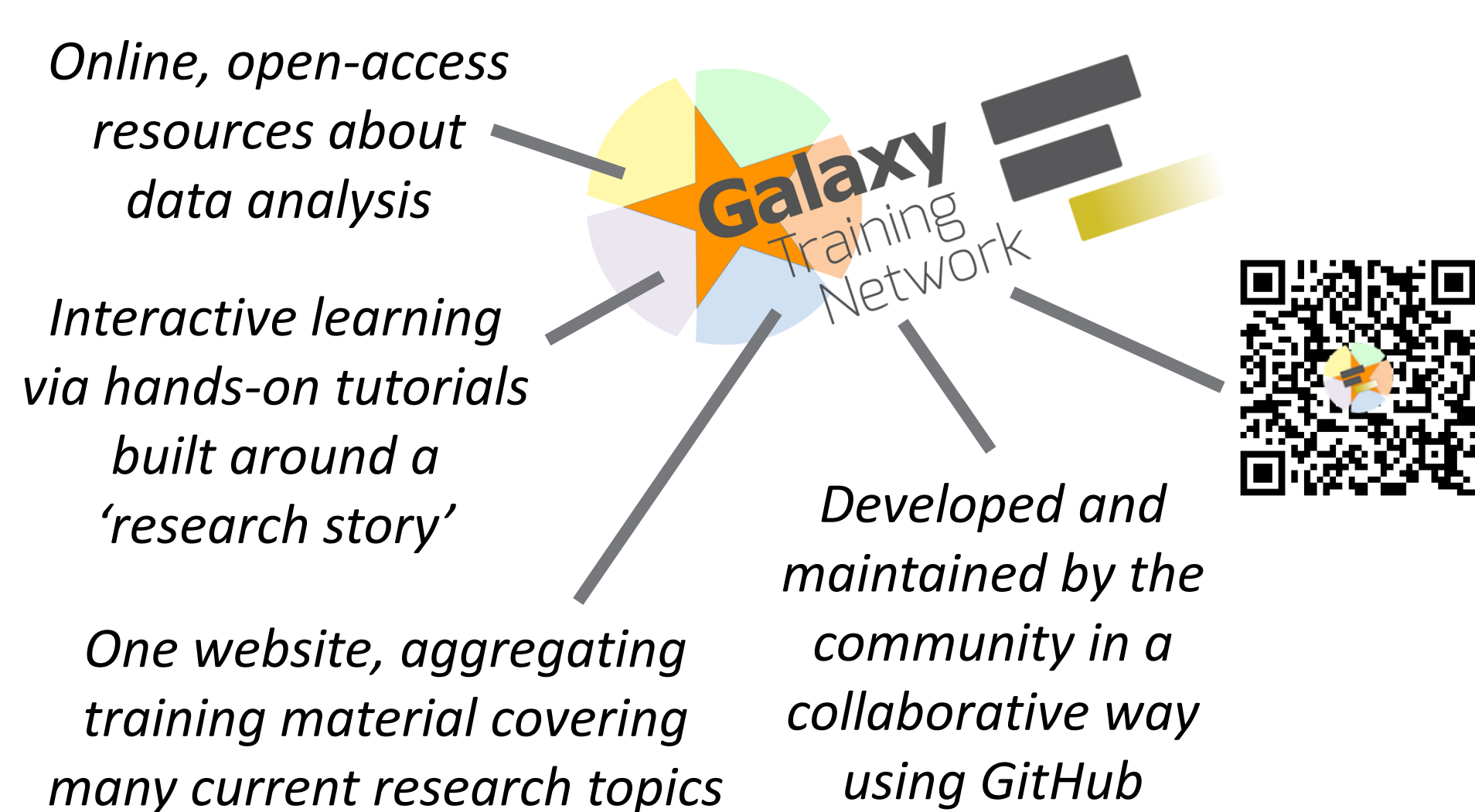


The **W4M** infrastructure will join the **usegalaxy.fr** initiative in 2020! More computational power resources, more data storage and more tools and data dynamic visualization – Watch this space!

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:



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