

4 Wm

Workflow4metabolomics

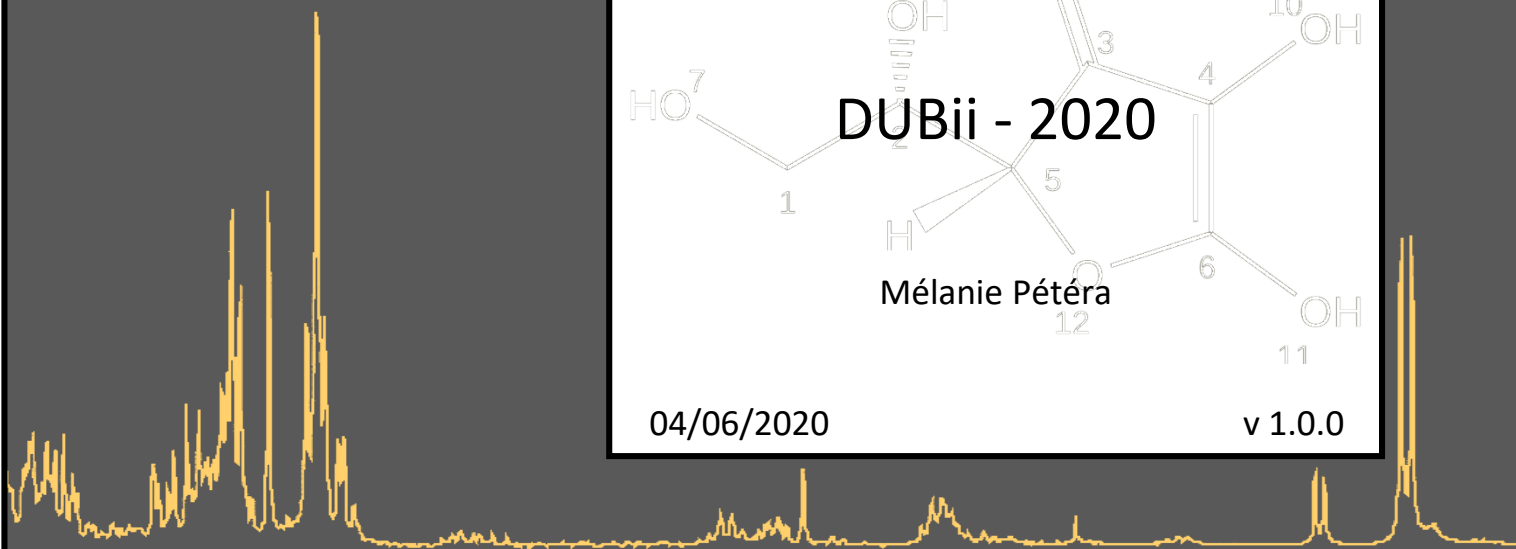


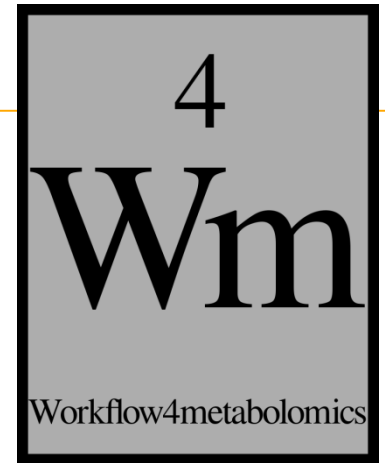
W4M



04/06/2020

v 1.0.0

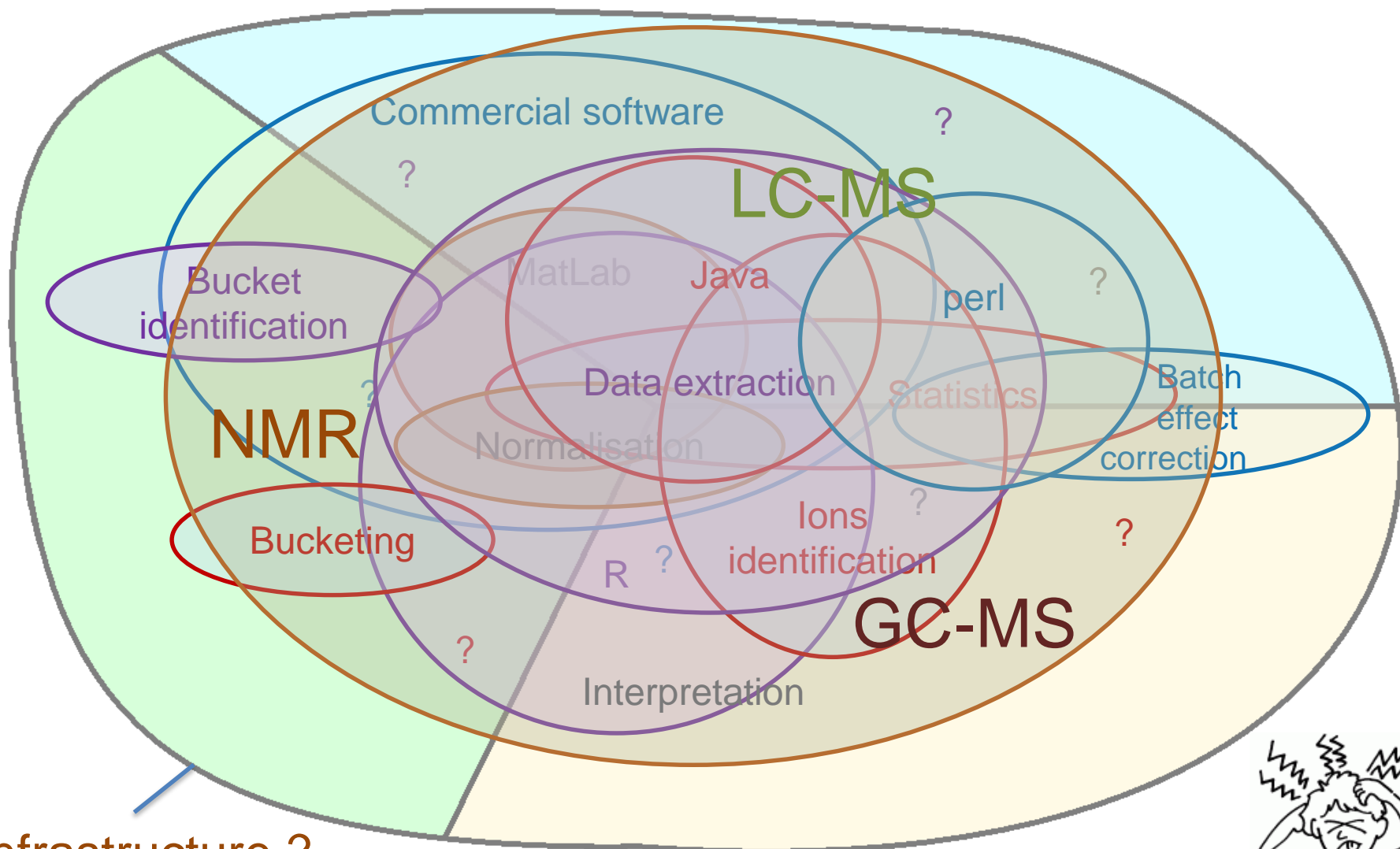




Workflow4Metabolomics – W4M

POURQUOI ?

Une multitude d'outils



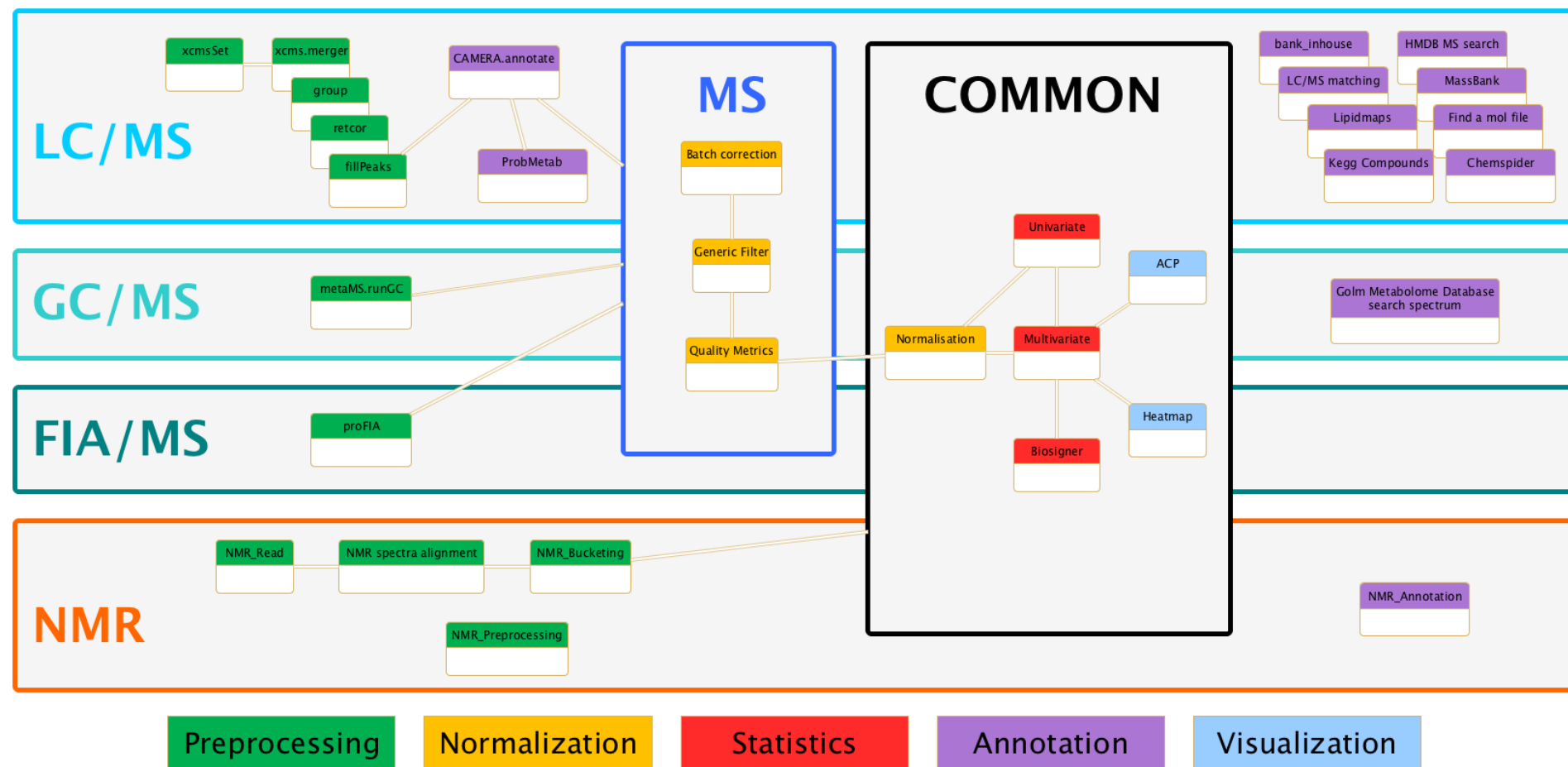
COMMENT ?

W4M – un travail collaboratif



- ❖ Un partenariat entre plusieurs structures dont MetaboHub et l'IFB (infrastructures d'avenir)
- ❖ Développement d'outils autour de la métabolomique : RMN, MS
- ❖ Mise à disposition de ces outils pour pouvoir traiter les données « de A à Z »

Des outils mis en commun pour couvrir l'essentiel



Galaxy / Workflow4Metabolomics

Analyse de données Workflow Visualize Données partagées Aide Authentification et Enregistrement

Using 9%

Tools

search tools

Get Data

Collection Operations

Text Manipulation

WORKFLOW4METABOLOMICS

Get Data - Metabolomics

Preprocessing LCMS

Preprocessing FIAMS

Preprocessing GCMS

Preprocessing NMR

Quality processing MS

Quality processing ALL

Statistics ALL

Annotation LCMS FIAMS

Annotation GCMS

Annotation NMR

MSMS

Data handling ALL

Graph/Display Data

Workflows

All workflows

4
Wm
Workflow4metabolomics

Workflow4metabolomics

What you have read and accept the [Term for Use](#)

James Taylor died yesterday. Our dear @jxtx -> Galaxy began with you. We will make sure it continues. We have no words.

5:27 5:22 PM - Apr 3, 2018

376 people are talking about this

Current version: 1.5

Publication: Franck Giacomoni, Gildas Le Corguillé, M. Sharl Monsoor, Marion Landi, Pierre Pericard, Melanie Pétéra, Christophe Duperier, Marie Tisserand, Jean-François Franco, Jean-François Martin, Daniel Jacob, Sophie Schmitt, et al. Workflow4metabolomics: A collaborative research infrastructure for computational metabolomics. *Bioinformatics* (2018) 34(10):1093-1100. doi:10.1093/bioinformatics/btu813

Changelog

MS COMMON

MS

COMMON

History

Rechercher des données

imported: DUBii_backup1

14 shown, 36 hidden

984.15 MB

139: xset.merged.grou	eye	edit	delete
p.dataMatrix.tsv			
138: xset.merged.grou	eye	edit	delete
p.variableMetadata.tsv			
137: xset.merged.grou	eye	edit	delete
pChromPeaks.plotChro			
mPeakDensity.pdf			
136: xset.merged.grou	eye	edit	delete
pChromPeaks.RData			
135: xset.merged.samp	eye	edit	delete
leMetadata.tsv			
134: xset.merged.RDat	eye	edit	delete
a			
115: sacarine.raw.xset.log.txt			x
a list with 9 items			
114: sacarine.raw.xset.RData			x
a list with 9 items			
113: BPL.pdf	eye	edit	delete
112: TIC.pdf	eye	edit	delete
111: sampleMetadata_c	eye	edit	delete
completeMetadata.t			
09: sacarine.raw.RData			x
set with 9 items			

What we need as developers

Easy integration of tools

Multi-language

Collaborative development

Open-source

Possibility of link with external ressources

What we need as users

GUI

Ergonomics

Parameter completeness

Modularity

Data & workflow sharing

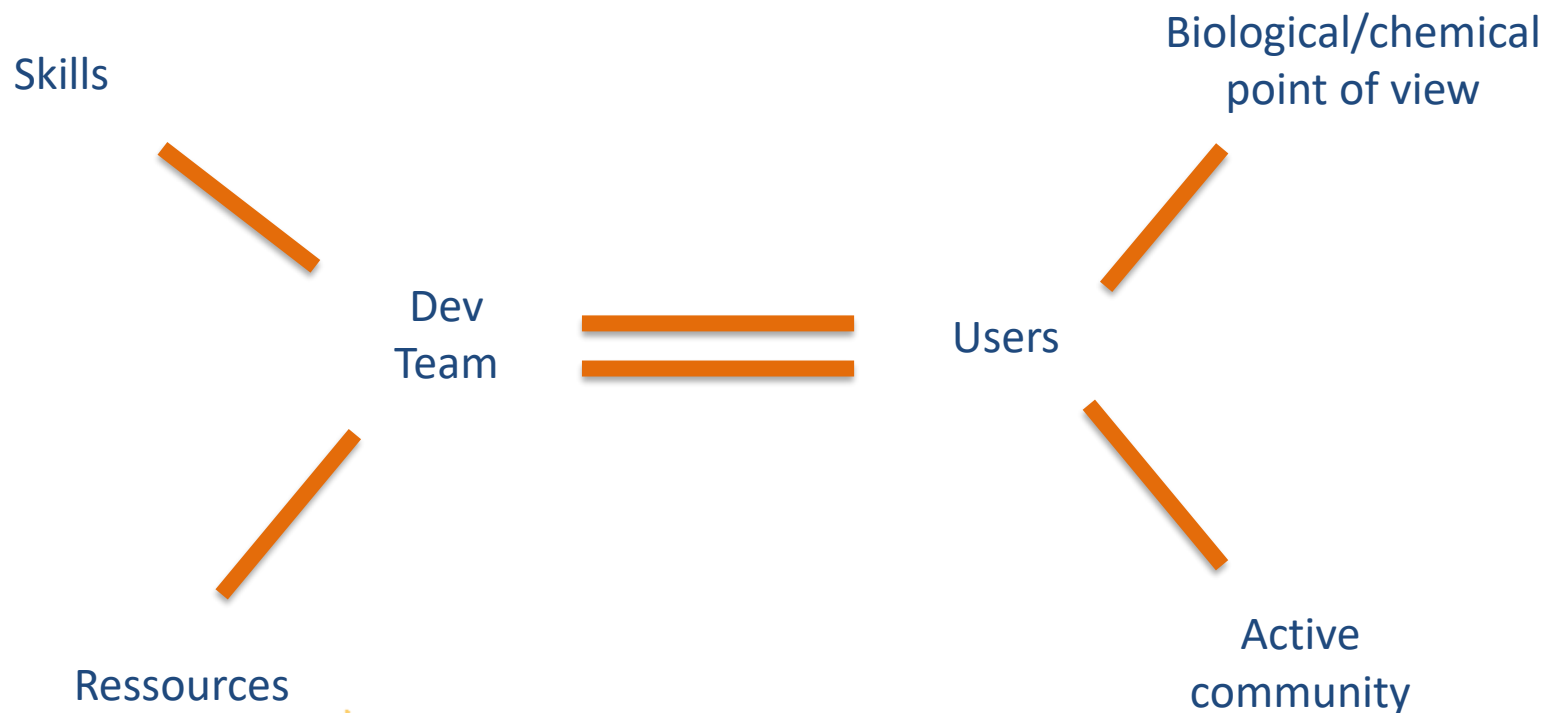
Possibility of new tools' integration

UNE COMBINAISON GAGNANTE !

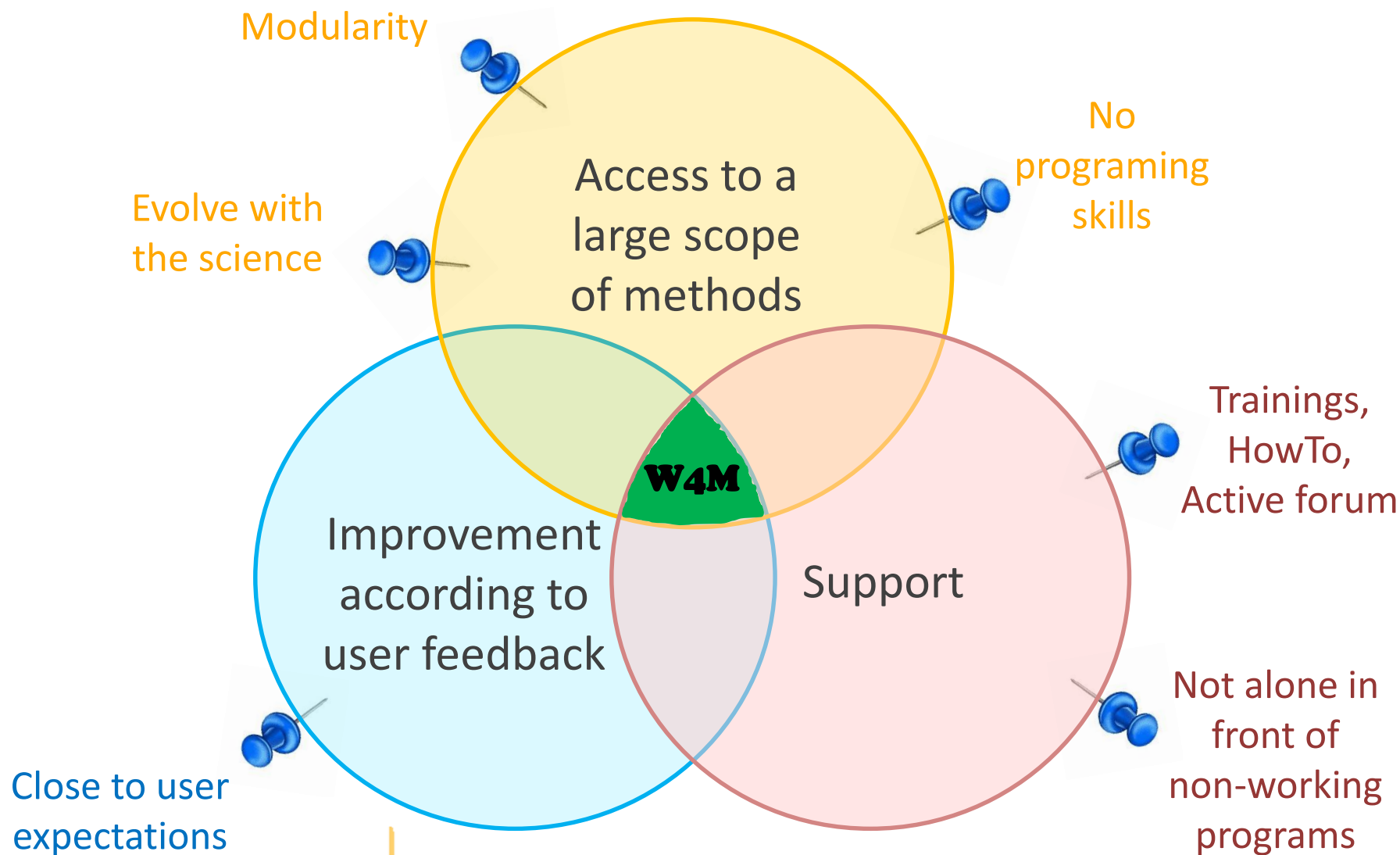
La chimie de W4M

Our equation

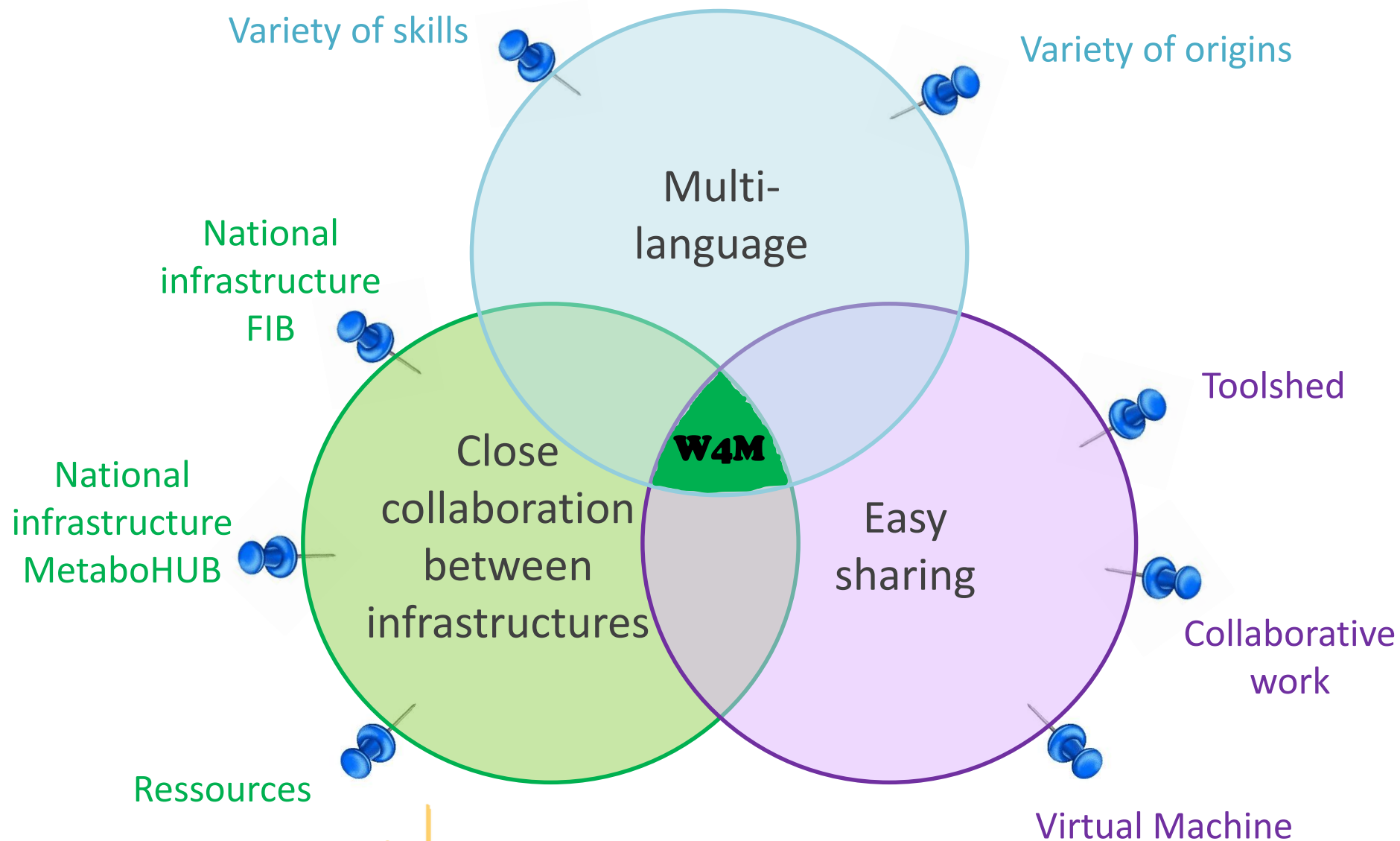
Easy access to existing tools + Development of new tools + Easy handling for users → **W4M**



Efficace pour les utilisateurs



Efficace pour les développeurs



Pour aller plus loin

<https://workflow4metabolomics.org/>

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Bioinformatics, 2015, 1-3
doi:10.1093/bioinformatics/btu213
Advance Access Publication Date: 19 December 2014
Applications Note

OXFORD

Gene expression

Workflow4Metabolomics: a collaborative research infrastructure for computational metabolomics

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Abstract
Summary: The complex, rapidly evolving field of computational metabolomics calls for collaborative infrastructures where the large volume of new algorithms for data pre-processing, statistical analysis and annotation can be readily integrated whatever the language, evaluated on reference datasets and chained to build ad hoc workflows for users. We have developed Workflow4Metabolomics (W4M), the first fully open-source and collaborative online platform for computational metabolomics. W4M is a virtual research environment built upon the Galaxy web-based platform technology. It enables ergonomic integration, exchange and running of individual modules and workflows. Alternatively, the whole W4M framework and computational tools can be downloaded as a virtual machine for local installation.
Availability and implementation: <http://workflow4metabolomics.org> homepage enables users to open a private account and access the infrastructure.
W4M is developed and maintained by the French Bioinformatics Institute (IFB) and the French Metabolomics and Fluxomics Infrastructure (MetaboHUB).
Contact: contact@workflow4metabolomics.org

1 Introduction
Metabolomics, the high throughput analysis of small molecules in biological samples, heavily depends on data pre-processing, statistical analysis and chemical and biological annotation, which are complex, transdisciplinary processes involving both computation

volume of proposed algorithms written in various languages, making their evaluation by the bioinformatics community (including reviewers) and their chaining within ad hoc workflows by experimenters difficult (Smith et al., 2013).
A few user-oriented online platforms for metabolomics data pre-

Downloaded from <http://bioinformatics.oxfordjournals.org/> at UPMC on March 23, 2015



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Create, run, share, publish, and reference your LC-MS, FIA-MS, GC-MS, and NMR data analysis workflows with the Workflow4Metabolomics 3.0 Galaxy online infrastructure for metabolomics



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ABSTRACT

Metabolomics is a key approach in modern functional genomics and systems biology. Due to the complexity of metabolomics data, the variety of experimental designs, and the multiplicity of bioinformatics tools, providing experimenters with a simple and efficient resource to conduct comprehensive and rigorous analysis of their data is of utmost importance. In 2014, we launched the Workflow4Metabolomics (W4M, <http://workflow4metabolomics.org>) online infrastructure for metabolomics built on the Galaxy environment, which offers user-friendly features to build and run data analysis workflows including preprocessing, statistical analysis, and annotation steps. Here we present the new W4M 3.0 release, which contains twice as many tools as the first version, and provides two features which are, to our knowledge, unique among online resources. First, data from the four major metabolomics technologies (i.e., LC-MS, FIA-MS, GC-MS, and NMR) can be analyzed on a single platform. By using three studies in human physiology, alga evolution, and animal toxicology, we demonstrate how the 40 available tools can be easily combined to address biological issues. Second, the full analysis (including the workflow, the parameter values, the input data and output results) can be referenced with a permanent digital object identifier (DOI). Publication of data analyses is of major importance for robust and reproducible science. Furthermore, the publicly shared workflows are of high-value for e-learning and training. The Workflow4Metabolomics 3.0 e-infrastructure thus not only offers a unique online environment for analysis of data from the main metabolomics technologies, but it is also the first reference repository for metabolomics workflows.

