



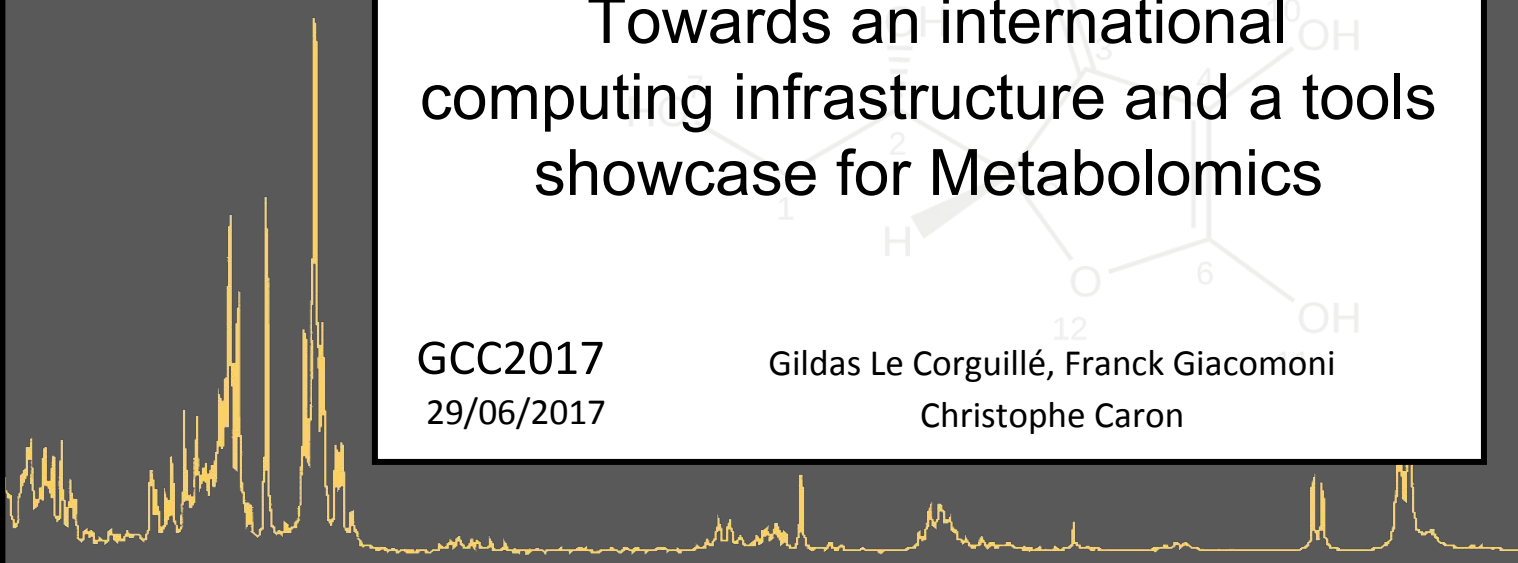
4  
Wm

Workflow4metabolomics

# Towards an international computing infrastructure and a tools showcase for Metabolomics

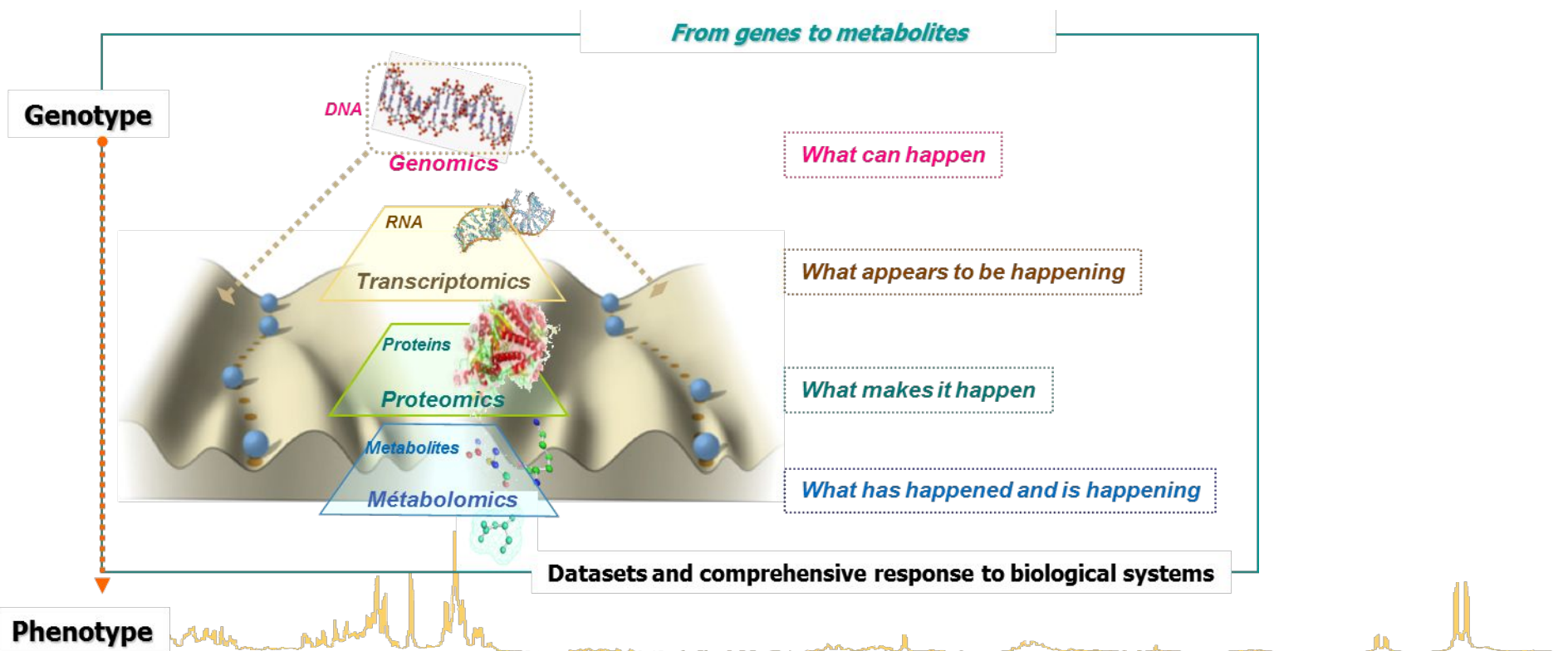
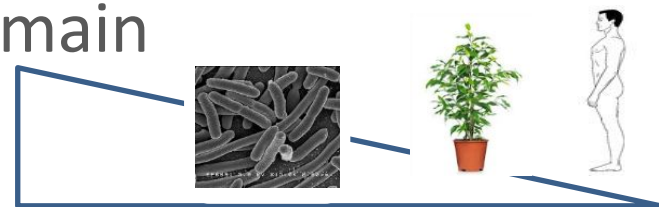
GCC2017  
29/06/2017

Gildas Le Corguillé, Franck Giacomoni  
Christophe Caron



# Biological context

- Identification and quantification of small molecules from the metabolism (metabolites)
- the most recent -omics research domain



# Metabolomics: a data driven approach

name	namecustom	mz	mzmin	mzmax
M100T183	M100.07529T183	100.075290217332	100.073962458109	100.075856347639
M101T64	M101.017412T64	101.017411813327	101.016363119337	101.025598611889
M101T1090	M101.094497T1090	101.094497373251	101.093825596321	101.094931330369
M102T67	M102.121467T67	102.121466917005	102.118620434328	102.128045805211
M103T60	M103.032369T60	103.032369394794	103.031358949596	103.040632681061
M103T61	M103.120075T61	103.120074855461	103.118630961785	103.129325340649
M104T1162	M103.950053T1162	103.950052934034	103.948946676433	103.95133690961
M104T60	M104.037434T60	104.037433793914	104.036015958492	104.046229685927
M104T47	M104.100665T47	104.100665065741	104.099665732044	104.108679356773
M104T88	M104.095422T88	104.095422407145	104.093036006622	104.100116358936
M104T42	M104.195599T42	104.195598628802	104.187807623186	104.197644370905
M105T61	M105.045229T61	105.045228536653	105.036480671616	105.046334818564
M105T242	M105.069935T242	105.069934637469	105.06894296829	105.071143736243
M105T48	M105.103611T48	105.103611067744	105.102427529644	105.111698113321

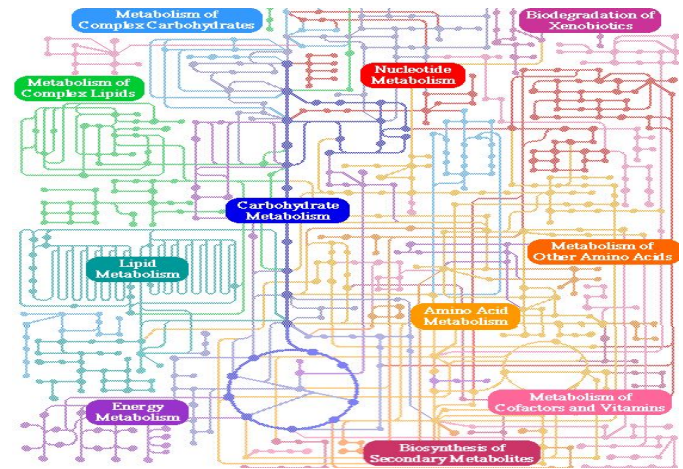


Interpretation

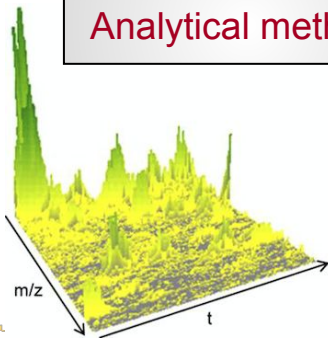
Identification

Statistical analysis

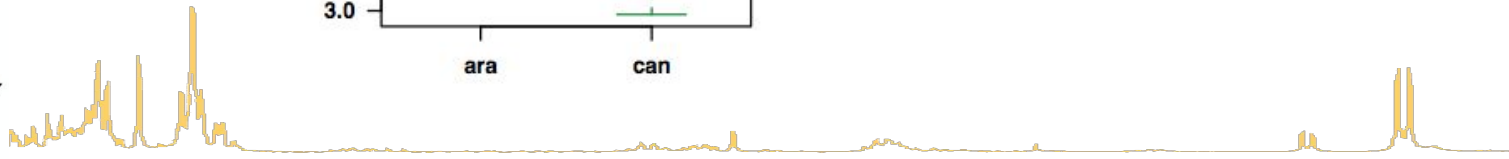
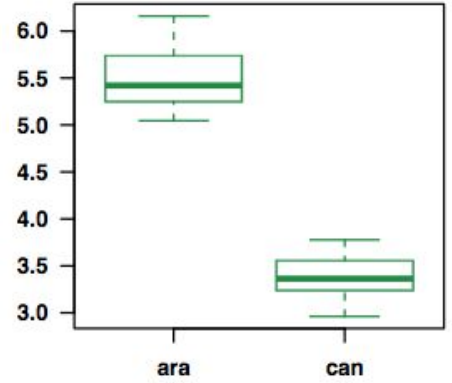
Data extraction



Analytical methods



M585T579  
RF







# Once upon a time... W4M

2012 - First tools

2013 - First talk at JOBIM - Toulouse

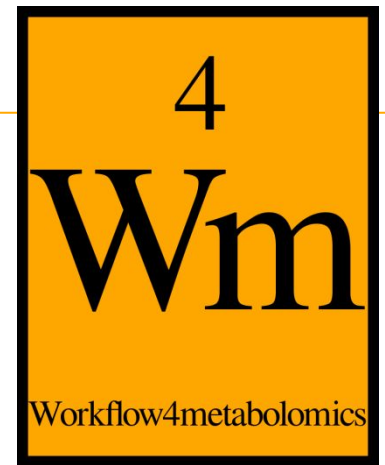
2013 - First [lightning] talk at GCC2013 - Oslo

2017 - We're back!



The W4M Community





# The W4M environment



# A main public instance

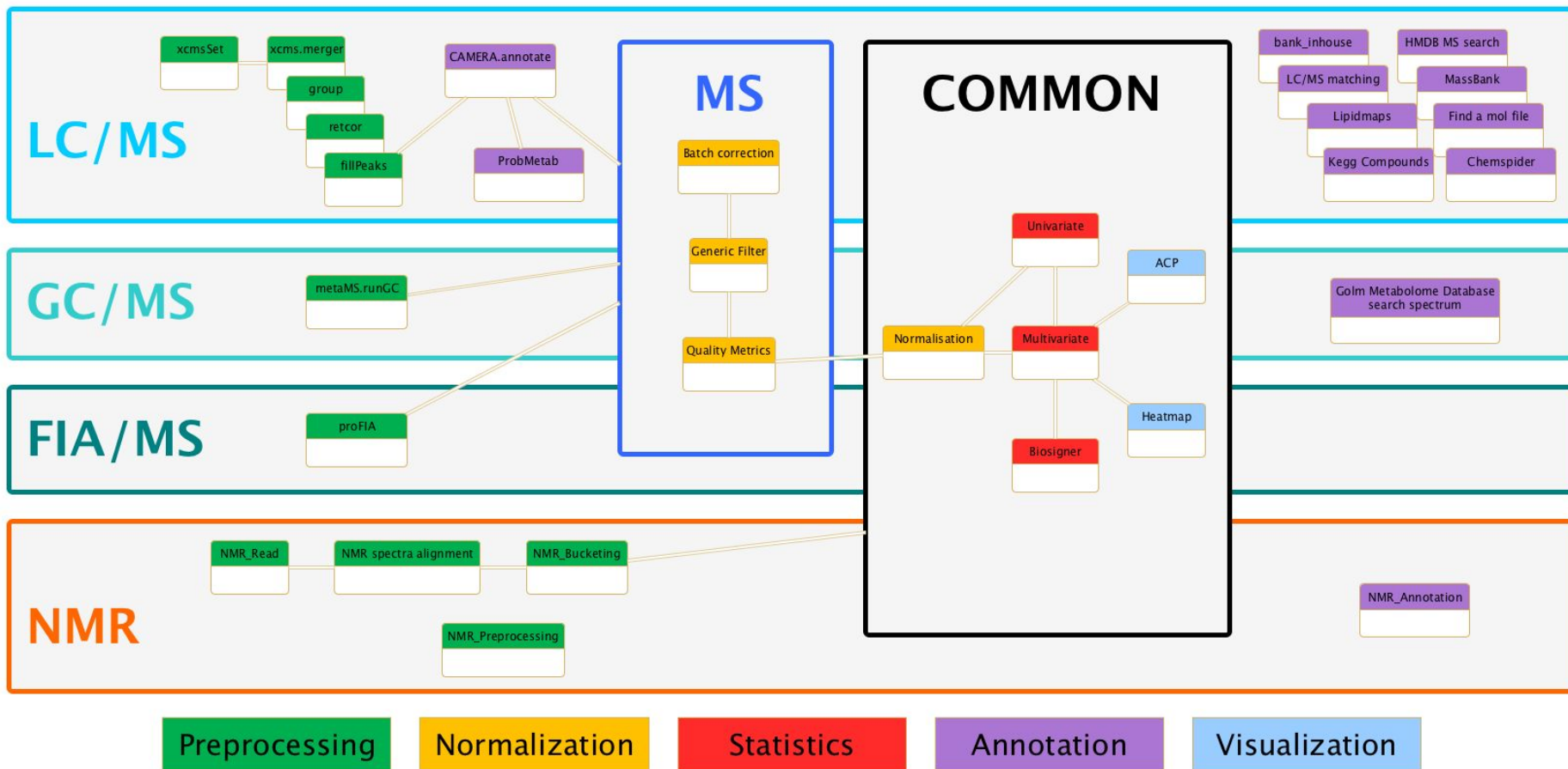
http://workflow4metabolomics.org

800 accounts  
25 000 jobs/year

19 related papers

HelpDesk [support@workflow4metabolomics.org](mailto:support@workflow4metabolomics.org)

# Tools



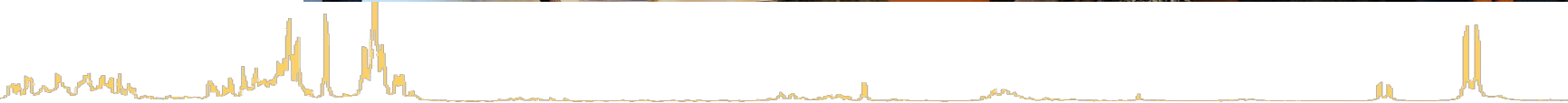
36 tools





## Workflow4Experimenters

- 3 sessions since 2014
- 10 Trainers for 20 Trainees
- “Bring your own data” tutoring sessions



# DOI

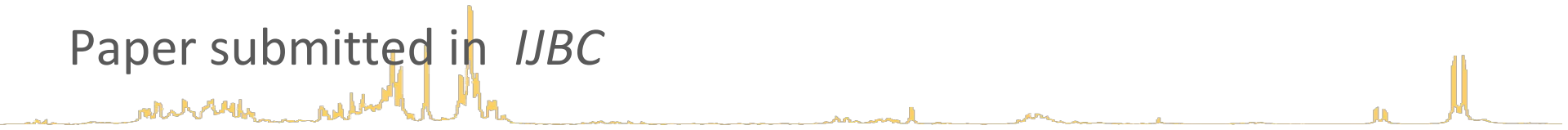


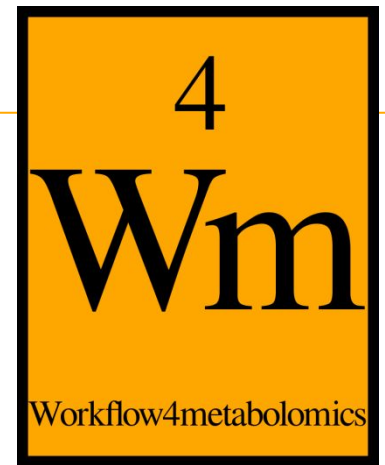
W4M provides DOI to reference histories and workflow usable in papers



[http://workflow4metabolomics.org/referenced\\_W4M\\_histories](http://workflow4metabolomics.org/referenced_W4M_histories)

Paper submitted in *IJBC*



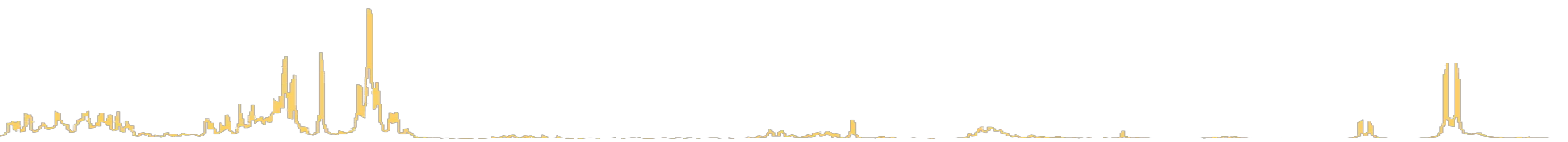
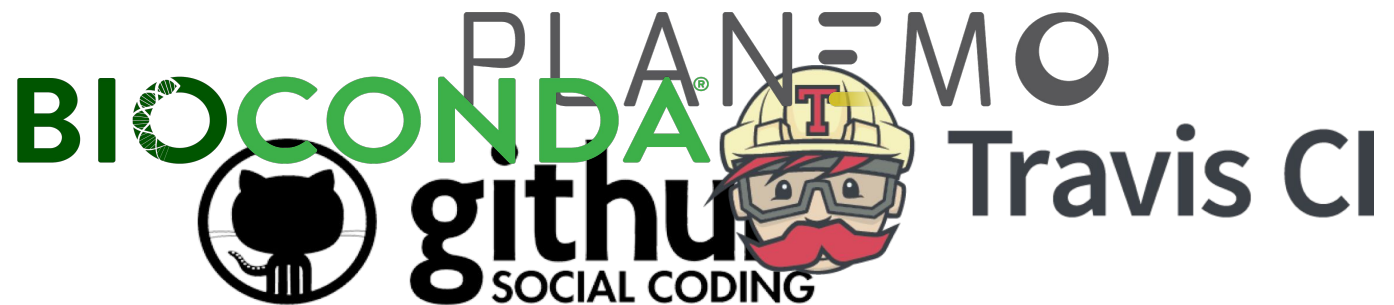


# BACK OFFICE



## Developments

- 15 developers from 7 laboratories
- Stick to IUC standards
- A GitHub: [github.com/workflow4metabolomics](https://github.com/workflow4metabolomics)
- Conda / Planemo / TravisCI



# GET: An Open Project

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All public W4M tools are distributed:



Dev:

[github.com/workflow4metabolomics](https://github.com/workflow4metabolomics)



Wrappers: on main Galaxy ToolShed

[toolshed.g2.bx.psu.edu/groups#/175812cd7caaf439](https://toolshed.g2.bx.psu.edu/groups#/175812cd7caaf439)



VM: with the most common W4M tools

[workflow4metabolomics.org/virtual-environments](https://workflow4metabolomics.org/virtual-environments)



Docker/Docker: A Galaxy Flavor

```
docker run -d -p 8080:80 workflow4metabolomics/galaxy-workflow4metabolomics
```



# PUSH: Contribution

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The main W4M instance as a Showcase

Hosting on W4M main instance

Quality standards (IUC Standard)



Advanced mode

Integration in our reference workflows

Follow your exchange formats between tools

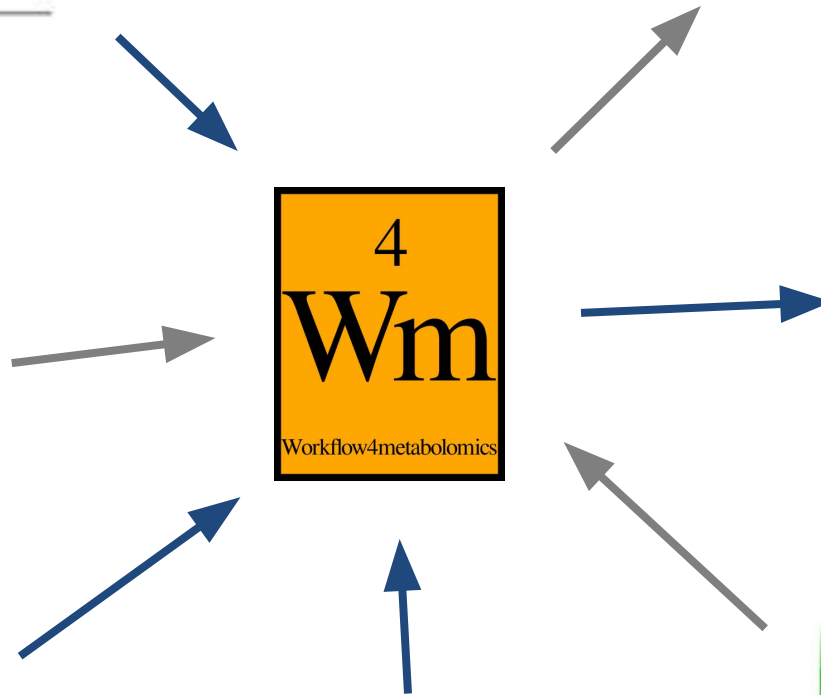
Collaboration mode if help is needed

However, the support must be done by the developers themselves

# Contribution in progress



MetaboFlow



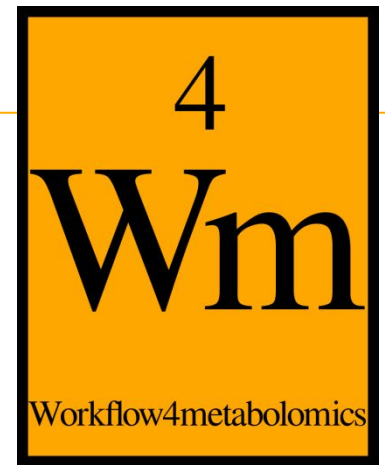
# Galaxy Training Network



 **Metabolomics lcms preprocess**  **work-in-progress**

#355 opened 12 days ago by lecorguille





# PERSPECTIVE



# Next steps

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- Visualization



- Interoperability



MetaboLights

- Trainings - e-Learning (2018)

- MOOC4Metabolomics

- Open Course 'e-Bioinformatics4Metabo'



UNIVERSITÉ DE  
RENNES 1

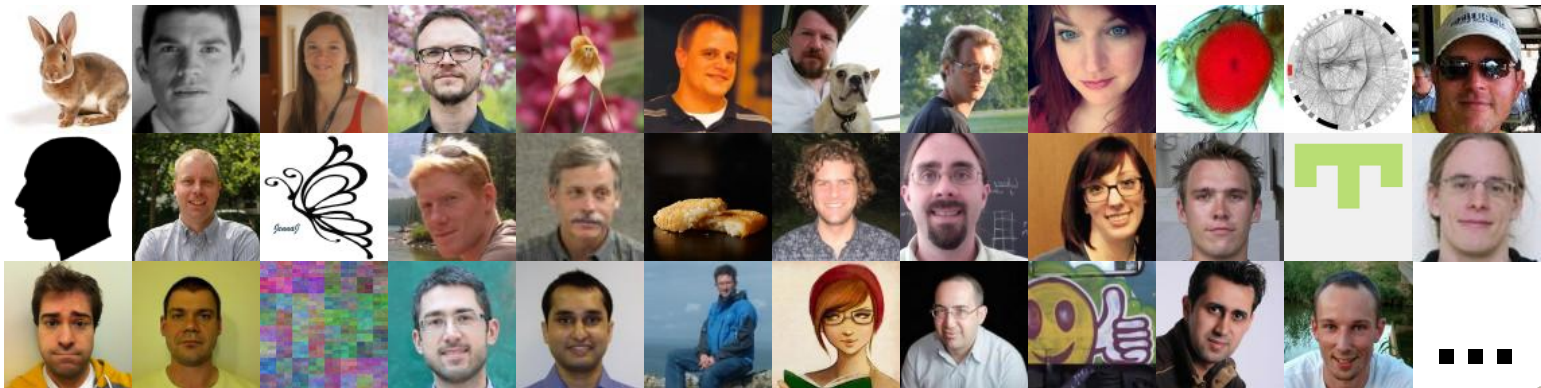


Réseau Français de Métabolisme et Biométabolisme





MERCI !



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