

# IFB Galaxy Day

## December 4th 2013

« Galaxy and the metabolomic  
analysis universe. »

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# A workflow for metabolomics

- ❖ Goals of the project :
  - Builds a workflow and preconfigurate workflows for metabolomic data analysis
  - Target(s) : Chemists, Biologists, Scientists of metabolomic field with different abilities level (beginner to expert)
- ❖ **Strengths** : *Galaxy a scientific web platform, knowledge*
- ❖ **Weaknesses** : no implementation exists
- ❖ **Opportunities** : *Collaboration / shared between 2 teams*
- ❖ **Threats** : Is Galaxy the right tool? Is the community ready?

# Common practices involved in :

## ❖ *Environment :*

- Same VM with OS and Galaxy version
- Two Galaxy instances : Dev + Prod
- « Think workflow » as soon as possible
- Common tools integration rules

## ❖ *Integration steps*

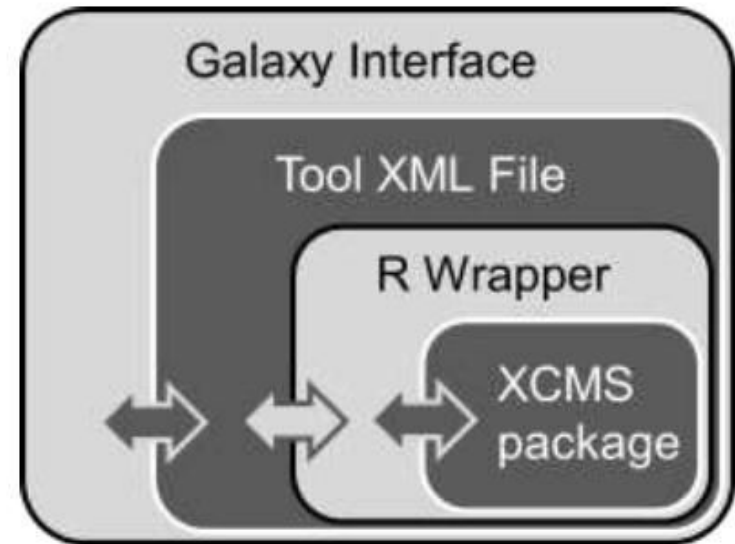
- « **Tool Definition File** » template / mandatory parts (Help)
- Data set proposal in « Help » part or on « pages »
- Shared practices in dev steps

# Common practices involved in :

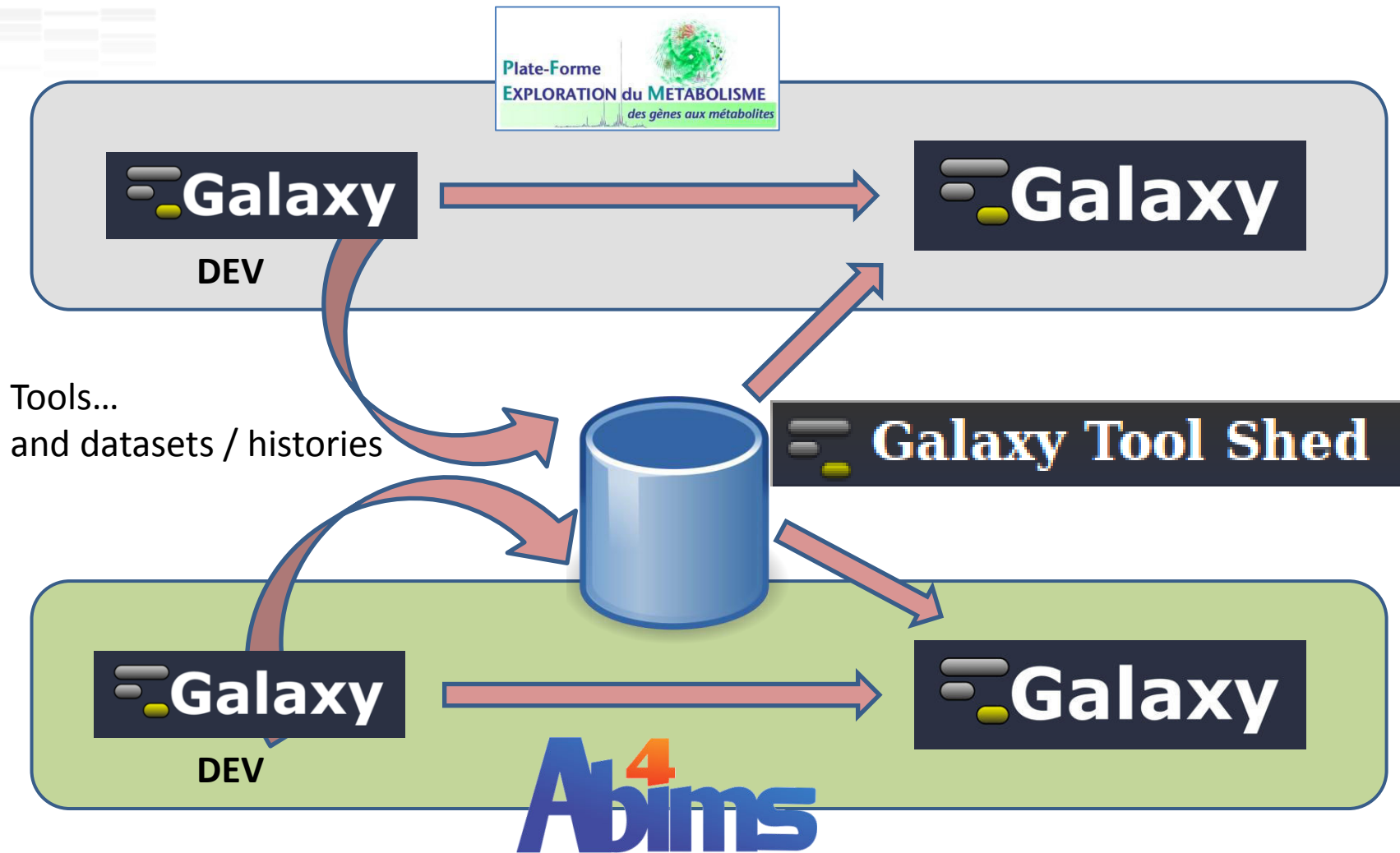
- ❖ Quality level (before production):
    - Working tool (functional level)
    - Ergonomy of parameters and uses : tested by final user
    - Writting « HELP » based on common template
      - Citations
      - Name of authors
      - Workflow position (upstream / downstream tools)
      - Input file(s) / parameter(s) / output file(s) descriptions
      - (Working example)
    - Short user guide
- ➔ Publications in IFB GT Galaxy Wiki

# Metabolomic Galaxy Experience

- ❖ R scripts wrapping
- ❖ JAVA wrapping
- ❖ Datatypes
  - Creation of RDATA
  - Adding « chemistry format »
- ❖ Own « Get Data »
  - Metabolomics produce huge datasets
    - « lib » mode to avoid massive upload

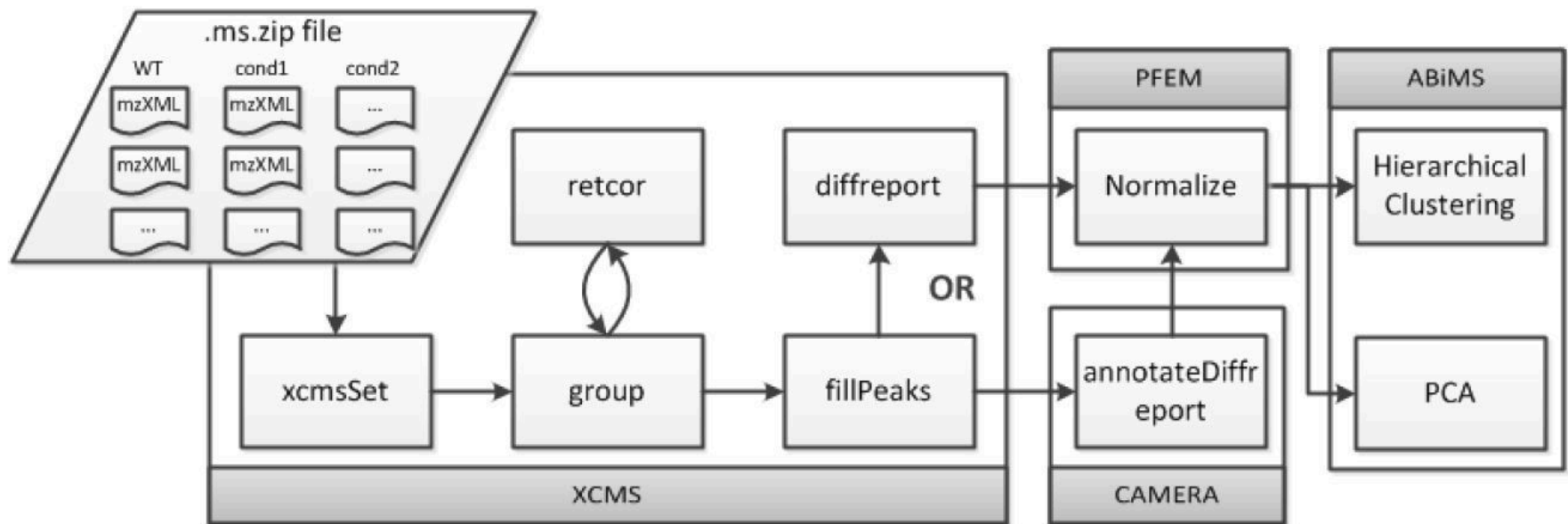


# A common toolshed



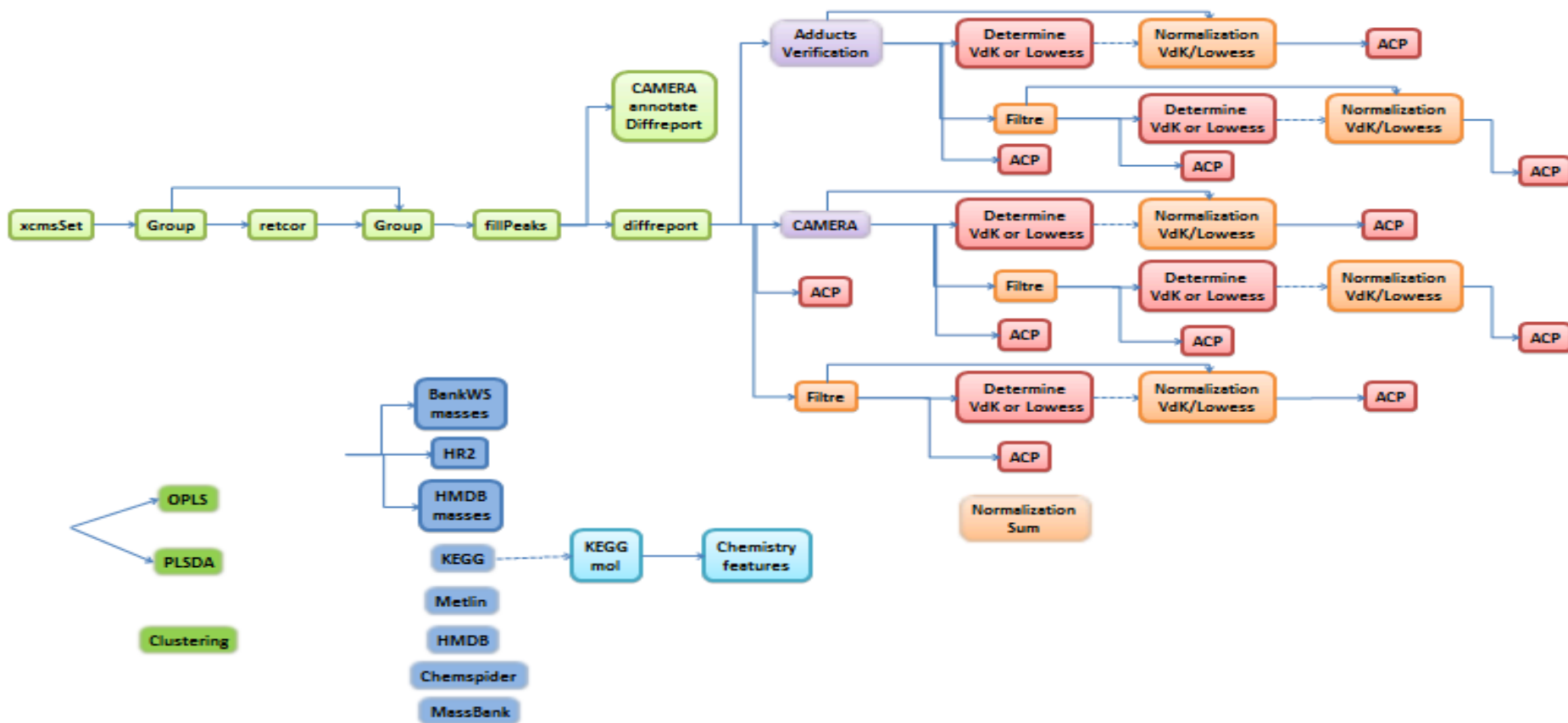
# Workflow4Metabo : a team project

- ❖ Galaxy is a federative tool :
  - bottom–up approach for projects
- ❖ Initial collaboration / first workflow
  - PF CNRS ABIMS / PF INRA PFEM



# Workflow4Metabo : a team project

❖ A few grants later :



BRIDGE    EXTRACTION    PEAKS ANNOTATION    DATA CORRECTION    QUALITY CONTROL    STATISTICS ANALYSIS    IDENTIFICATION



# Thank You!



**METABOMER**



Pierre PERICARD



Urszula CZERWINSKA



Sophie GOULITQUER



Gildas LE CORGUILLÉ



Christophe CARON



Mishari Monsoor



Estelle PUJOS-GUILLOT



Franck GIACOMONI



Marion LANDI



**FLAME**

**« Factory and Libraries for Automatic Metabolomic Exploration »**



Christophe DUPERIER



Jean-François MARTIN

