

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

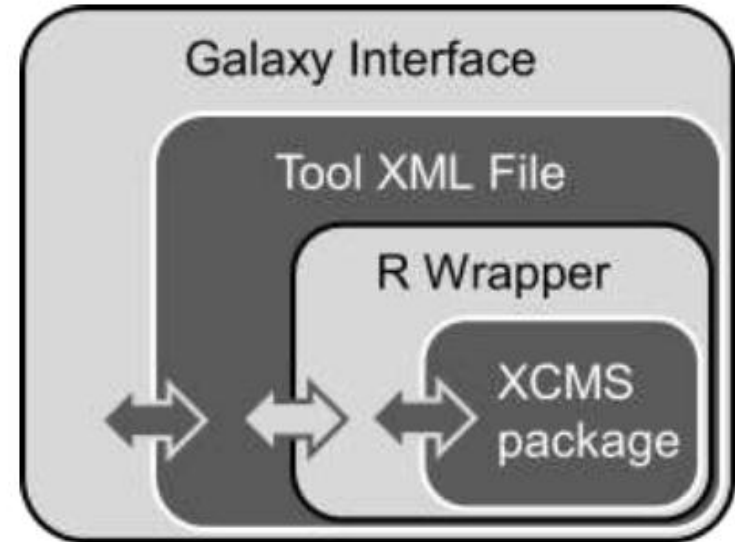
Common practices involved in :

❖ Quality level (before production):

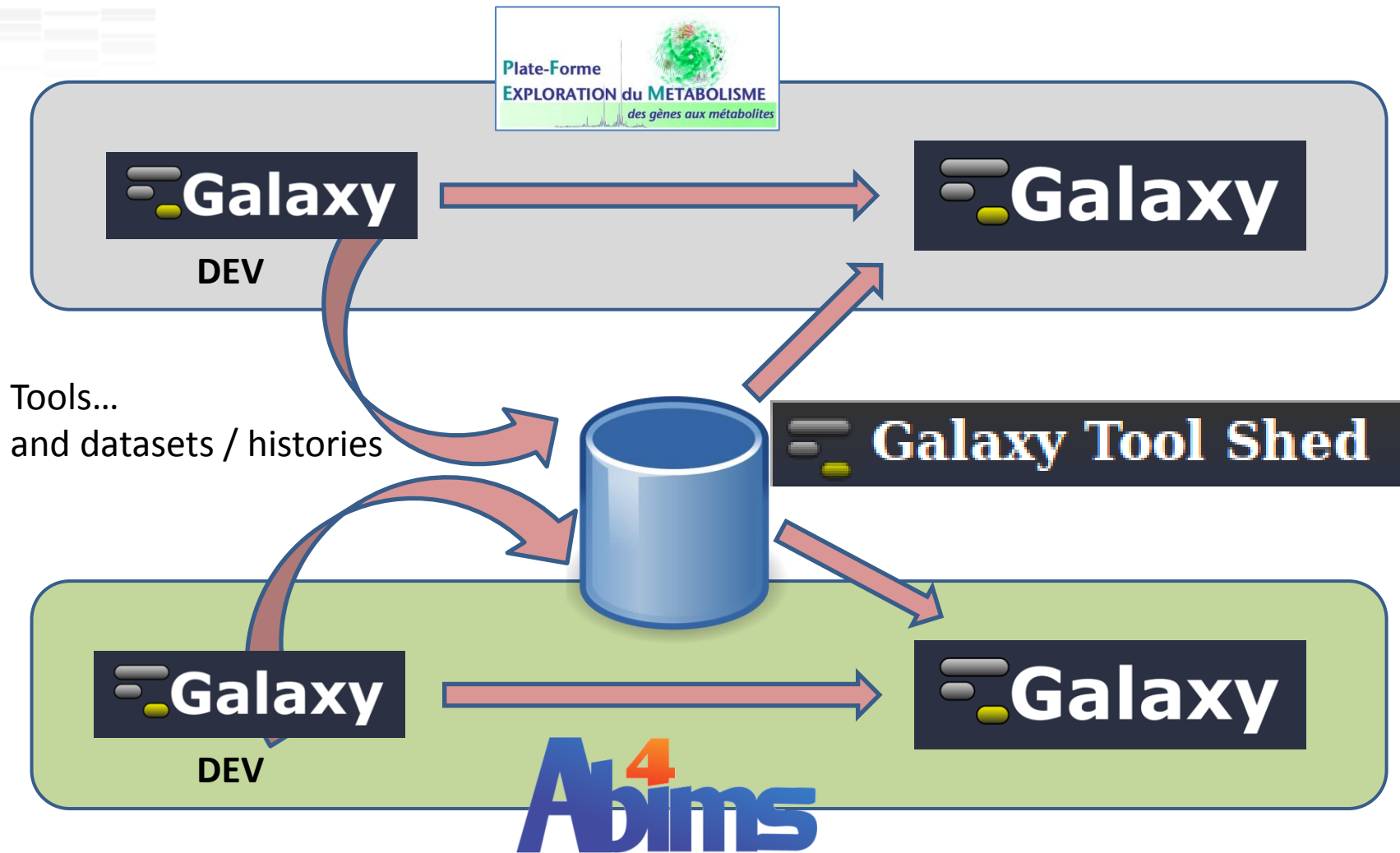
- Working tool (functional level)
 - Ergonomy of parameters and uses : tested by final user
 - Writting « HELP » based on common template
 - Citations
 - Name of authors
 - Workflow position (upstream / downstream tools)
 - Input file(s) / parameter(s) / output file(s) descriptions
 - (Working example)
 - 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

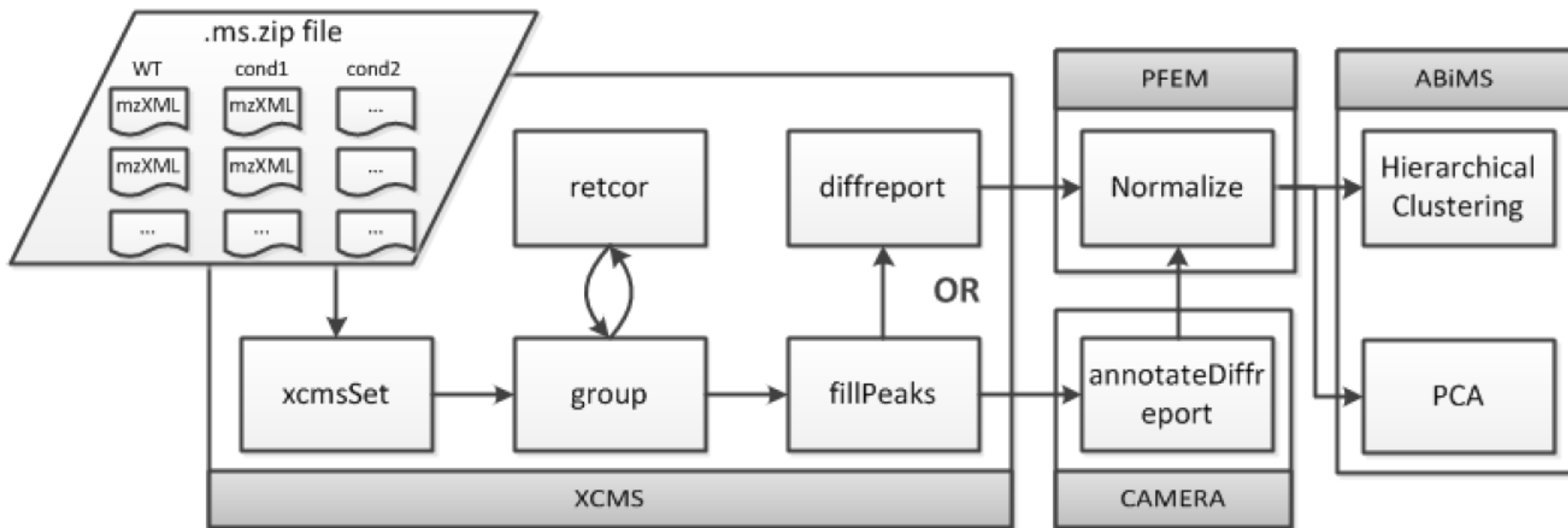


A common toolshed



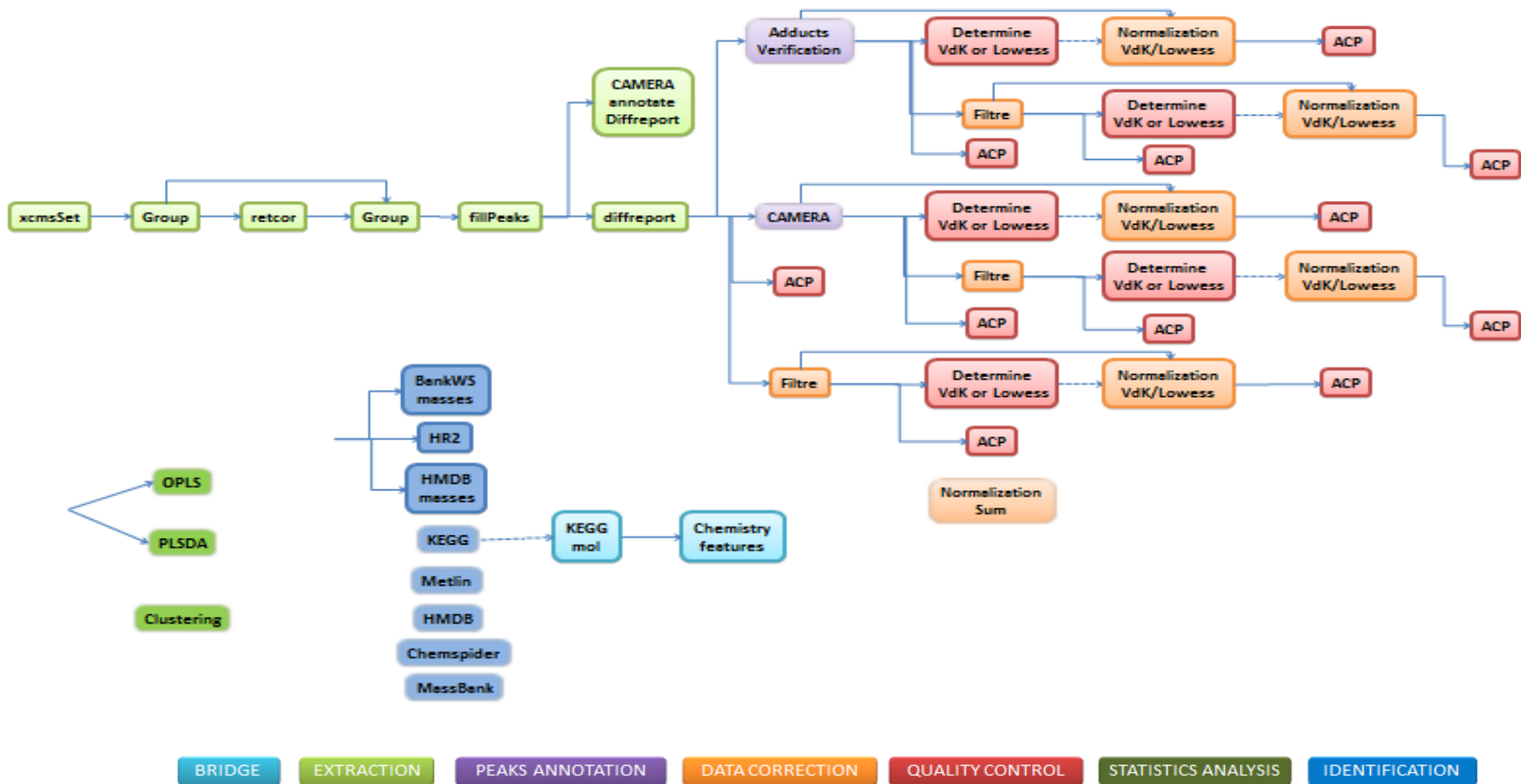
Workflow4Metabo : a team project

- ❖ 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 :



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

