

### MetaboHUB and RFMF: two tools at the service of metabolomics and fluxomics in France

Dominique Rolin, Floriant Bellvert, Justine Bertrand-Michel, Cécile Canlet, Richard Cole, Sophie S. Colombie, Catherine Deborde, Laurent Debrauwer, Marc Ferrara, Laetitia Fouillen, et al.

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# MetaboHUB and RFMF two tools dedicated to metabolomics and fluxomics in France

**Dominique Rolin** 

(rolin@bordeaux.inra.fr)

**MERLION Metabolomics** 

Workshop

http://www.metabohub.fr/en/

November 19 - 21, 2014









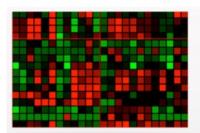


NUS Environmental Research Institute



19 NOV. / 21 NOV. - SINGAPOUR

### MERLION METABOLOMICS WORKSHOP SINGAPORE 2014



#### MERLION METABOLOMICS WORKSHOP SINGAPORE 2014

Developing Metabolomics Platform Technologies through Singapore-French Research Alliance

Date: 19 - 21 November 2014 Venue: University Town, National University of Singapore





### **Summary**

- \* New century and new scientific context
- Metabolomics a new tool for biology
- \* **RFMF**: a French bottom up initiative
- \* MetaboHUB: A French governmental top down initiative







### XXI century: new biology

The National Institutes of Health
The National Science Foundation
The Department of Energy



The National Research Coucil's Board on Life Science (2008-2009)

- 1- to examine the current state of biological research in the United States
- 2- recommend how best to capitalize on recent technological and scientific advances

# Report A New Biology for the 21st Century

http://www.nap.edu/catalog/12764.html

- Goals: 1- Propel science to a new level
  - 2- Provide solutions to pressing societal problems





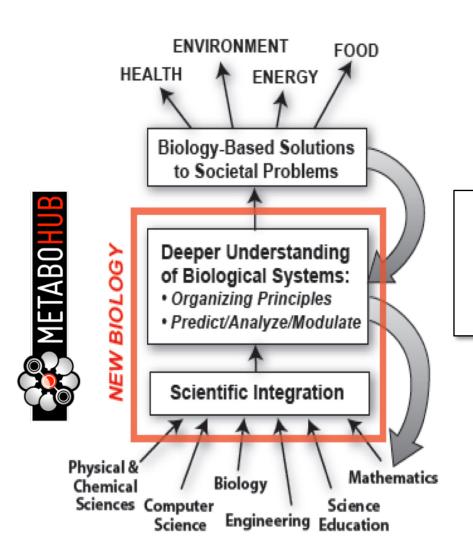


**Environment** 





### XXI century: new biology



MetaboHUB has been build according to the precepts laid down in this Report

Interconnected problems need
Interconnected solutions

The challenge cannot be met in isolation





# What do we mean by metabolomics and fluxomics?

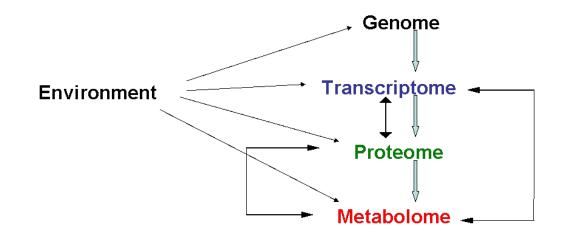
#### **Metabolome:**

all small molecules (metabolites) occurring in a biological system.

Stephen Oliver (1998, UK)

#### Fluxome:

All quantified metabolite fluxes occurring in a biological system.



#### **Metabolomics:**

Tools and strategy for determination of metabolite levels occurring in a biological system. and their changes over time as a consequence of stimuli

#### **Fluxomics:**

Tools and stratgy for determination of metabolite fluxes occurring in a biological system. and their changes over time as a consequence of stimuli

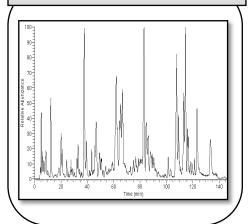




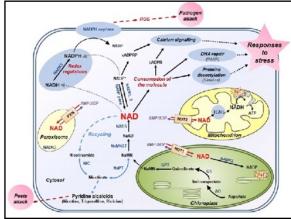
# What do we mean by metabolomics and fluxomics?

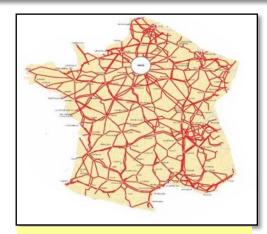
#### Metabolomics profiles

#### Targeted or non targeted



# Biological system: Cell Metabolic pathway map



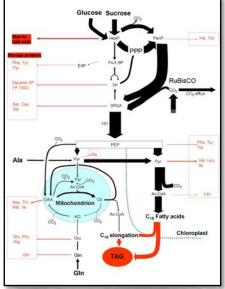


#### Car traffic



France = Road network

#### Metabolic flux analysis





Car traffic



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### Tools to build the future

**MetaboHUB** is a French governmental "**top down**" initiative aimed to set up a French Infrastructure devoted to the M & F in France



2013



2005

French Network for Metabolomics and Fluxomics

This is a typical "bottom up" initiative aimed at facilitating and promoting

sustainable development of the M &F in France



### RFMF Goals since 2005

### French Network for Metabolomics and Fluxomics

- Foster relationships between French researchers in M & F
- Promote and structure education and training in M & F
- Organize and support the organization of conferences in France
- Encourage through grants the participation of young researchers to national and international conferences
- Allocate funds mission or prizes for accomplished work in M & F

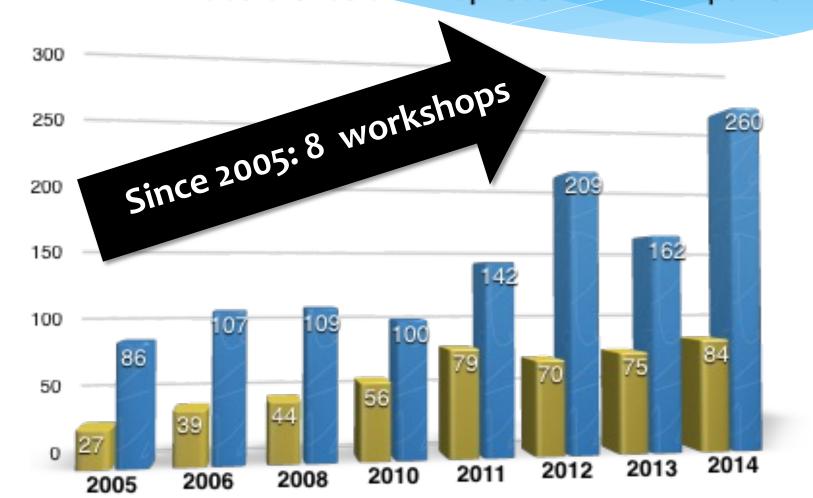




### **RFMF** Actions since 2005

A growing community with a geographic & thematic expansion

Laboratoires & Entreprises Participants







### **RFMF** Actions since 2005



#### 300 members connected by a mailing list and a Web site

2013: 136 messages were relayed on the mailing list mainly for job position



#### Since 2005: financial support to young scientists

2013: 15 travel grants (4300 euros)

2014: 18 travel grants (3730 euros)



#### Since 2013: Sponsoring the RFMF Junior

Pedagogic actions for Master students through a Master session during the annual workshop

#### Sponsoring collective research (15 Laboratories)

3 posters and 1 publication in Metabolomics

#### Organizing specialized workshop and round tables

on techniques, sofwares, procedures,



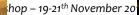
### 9 èmes Journées Scientifiques



RÉSEAU FRANÇAIS DE MÉTABOLOMIQUE ET FLUXOMIQUE

### June 2015 Villeneuve d'Ascq (Lille)

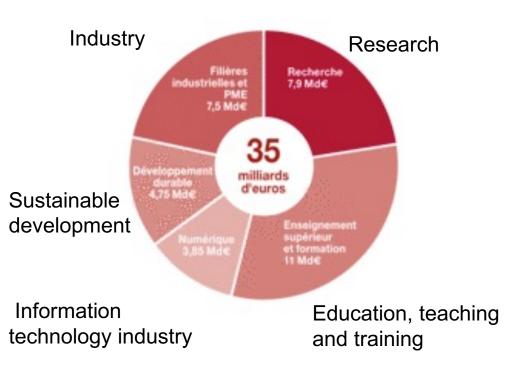






# MetaboHUB is a French governmental "top down" initiative FRENCH STRATEGY FOR RESEARCH AND INNOVATION Investment Program for the Future (PIA) (2009)



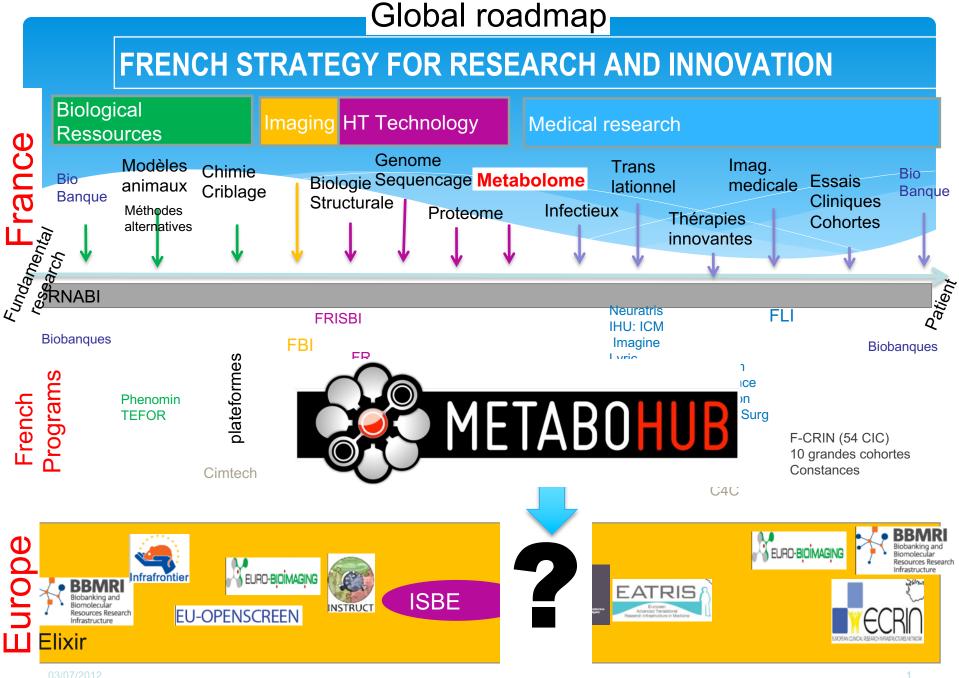


#### Selected areas (9)

Valorization of Research

Health and Biotechnology
Financing of companies
Transportation industries
Digital Economy
Energy and recycling economy
Urbanism and Property
Centers of excellence
Equal opportunities





catherine.chapel@recherche.gouv.fr

ESFRI= European Strategy Forum on Research Infrastructures



### MetaboHUB missions

## Creation world-class metabolomics knowledge infrastructure to contribute to science

Contribution to solve biological questions linked to pressing societal problems

(Food, Environment, Agriculture, Health, Biotechnology ...)

#### **MetaboHUB strategy and Challenges**

Generic technology development in the core programme
Providing services to the french community
Technology translation in application projects in collaboration with associate partners













### MetaboHUB challenges

### **Metabolomics and Fluxomics:**

### Much more complicated than a simple metabolite analysis

- Need a set of analytical methodologies
- Need a set of heavy and expensive equipment
- Need skills and specific competences
- Generate the concept of platforms
- Generate the concept of networking





**Lipidomics and the lipid world** 

Metabolite identification and quantification

Metabolic fingerprinting high density

Biomarker identification

Sample preparation

Biology expertise

Infrared technology

Apalytical

Data integration data mining

Data reduction

# INFORMATICS

Experimental Design

Metadata concept and database

LC-MS

NMR 1D-2D

Statistic analysis

Network analysis and modeling

Metabolomic flux quantification

Using stable isotopes for metabolomics



### MetaboHUB challenges

### Metabolomics is facing big technological and scientific challenges

#### For a huge world of applications

- Drug discovery and personal medicine
- Plant breeding and seed industry
- Nutrition and food industry
- Green and white biotechnology
- Environmental issues
- and much more...













#### What are the challenges?



### Metabolomics is facing a world of complexity

#### Metabolome definition

- is more conceptual than realistic
- generation of analytical challenges
- generation of methodological challenges
- generation of technological challenges
- generation of scientific challenges

Genetic input Environmental conditions

Metabolome

# We need to do some progress in the process of molecule identification and quantification How

- By using more efficient equipment
- By building spectral DB of reference molecules (MS, NMR)
- By developing exchangeable DB between machines
- Set up standardization procedures
- Developing new protocols that can be shared by all
- And much more...

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#### What are the challenges?

### Metabolomics is facing a world of complexity

#### Some progress are need in bioinformatics

- MetaDB (domain dependant)
- Spectral reference DB
- DB storage
- Data reduction
- Data interpretation
- Metabolic network analysis
- DB knowledge (domain dependant)
- etc...

### Part of the success go through regulatory and standardization issues

Especially to the transfer metabolomics technology to industry business





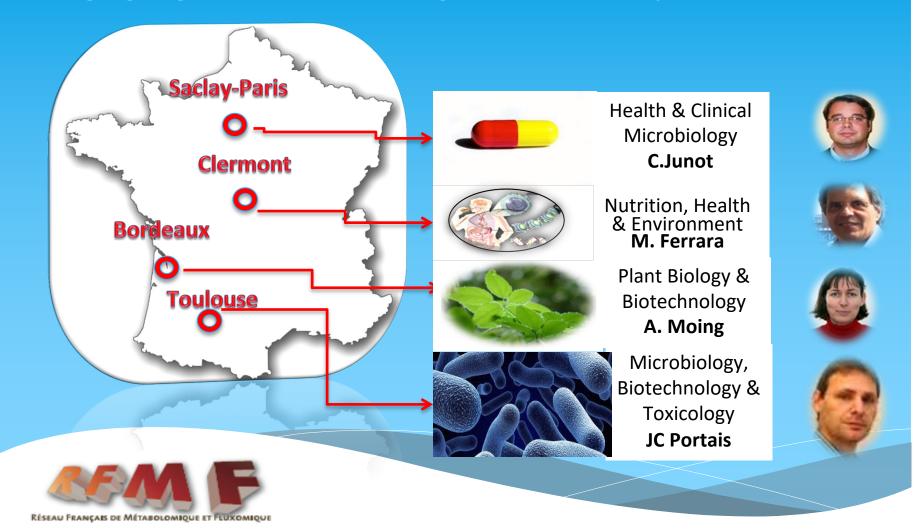






### **MetaboHUB** partners

Bringing together 4 outstanding metabolomics platforms





### A core facility with a wide range of analytical tools and competences

#### **7 NMR**

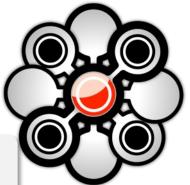


#### **Metabolic Flux** (Bio)chemistry







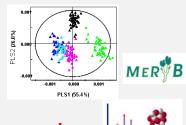


#### **Mass spectrometry**





**Bioinformatics, DB** & Biomathematics



11 specialized software's



#### **Robotics & HT devices**



Robots



8 servers

2 data bases



# A core facility with a wide range of analytical tools and competences

#### **NMR** Expertise

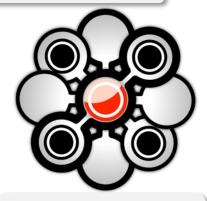


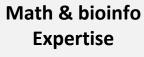




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# Platform leaders







#### **Lipidomics Expertise**













### How to meet the challenges?

Building term (2013-2016)
Science & technological developments

Service term (starting in january 2017)
Service & support for projects

**WP1 - Metabolomics** 

WP1 - Metabolomice Junot

**WP3 - Bioinformatics** 

WP3 - Bioinforma E. Lheneunot

**WP2 - Fluxomics** 

MLS - LINXOUIL JC. Portais

WP4 - Service

MP4 - Servi W. Eerrara

WP5 – Management WP6- Communication

WP5 – Management WP6- Commurco Santot





### How to meet the challenges?



WP1a: Metabolite identification and metabolome annotation (implement ation of spectral DB)

WP2a: Integrated tools for metabolic network reconstruction, visualization and modeling.





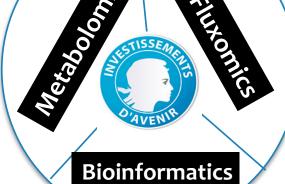
WP1b: Shared tools for lipidomics







WP1C: Tools for normalization and for quantitative MS-based metabolomics.



WP2C: Time and spatial re solution of the fluxome





WP3: Shared bioinformatics tools for data management and data mining











# Contribution of MetaboHUB to the MERLION Metabolomics Workshop

Untargeted metabolomic approaches and data mining tools for marker discovery in nutrition





Non targeted metabolomics for assessement of environmental exposure to contaminent and their biological efffects

Nutritional metabolomics as integrative understanding of metabolic desease development

Lipidomic analysis of palm oil variability

MS metabolomics and lipidomics for the study of rare deseases

Lipidomics: a key tool for human health

Biostatistic for biomarker discovery and phenotype prediction

**Human Health** 





Metabolic networking modelling and food Toxicity

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Date: 19 - 21 No.

Application of metabolomic finger printing for food quality assessments

A study on Honeybee losses: First insight into environmental interactions

Response of cloud microorganisms to atmosphere stresses: the case of study of cold shock

Comprehensive investigations of cellular meta bolic networks using 13c-fluxomics application to microbiology and biotechnology systems

notype prediction



Food Science

Biotechnology

**Environment** 





### Thank you for your attention











