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## 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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# Metabo**HUB** 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**



ANR-INBS-0010

MERLION Metabolomics Workshop – 19-21<sup>th</sup> November 2014 – National University of Singapore

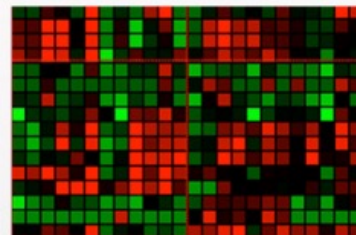


INSTITUT  
FRANÇAIS  
SINGAPOUR



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

- \* 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



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



The National Research Council'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>

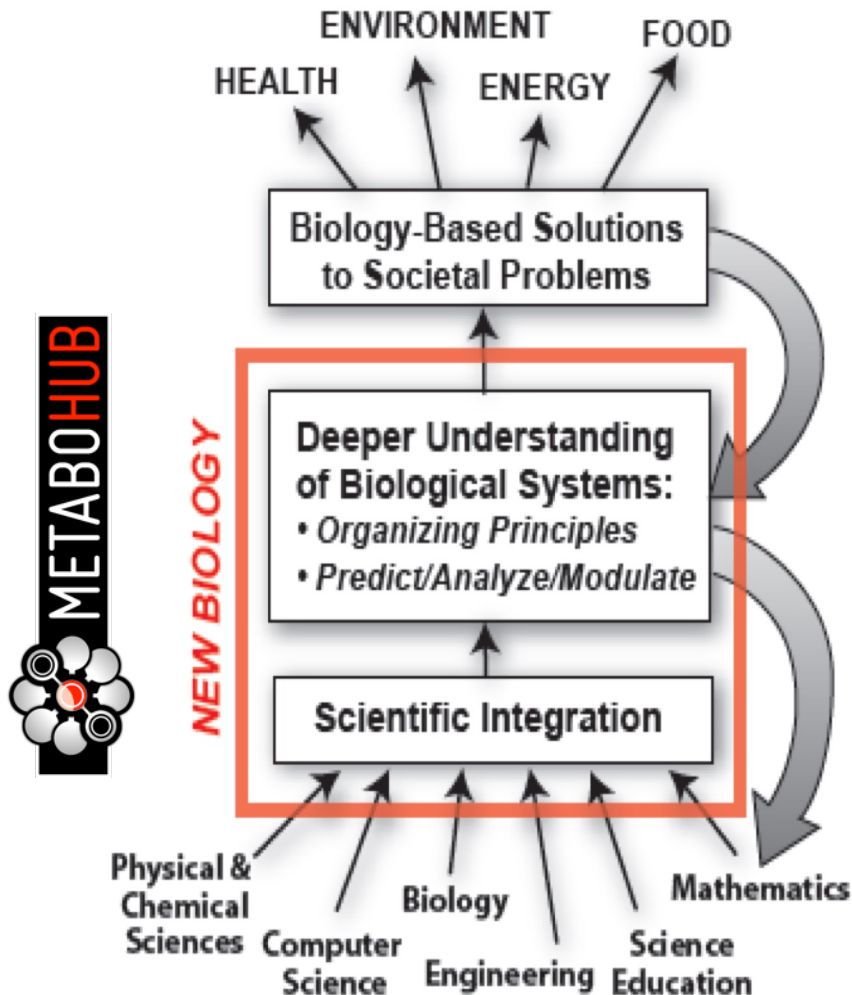
- Goals:**
- 1- **Propel science to a new level**
  - 2- **Provide solutions to pressing societal problems**

Human Health

Food Science

Energy

Environment



**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



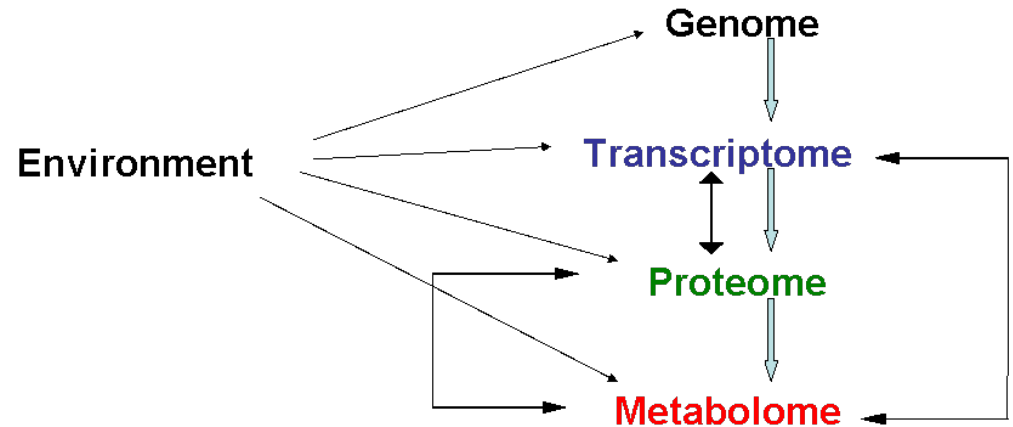
## Metabolome:

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

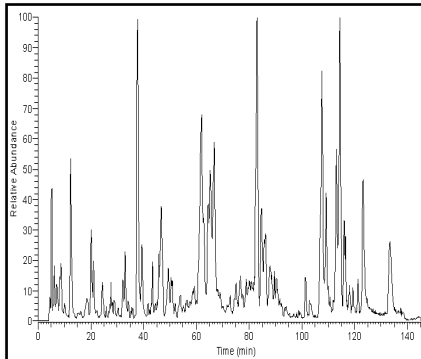
## Fluxomics:

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

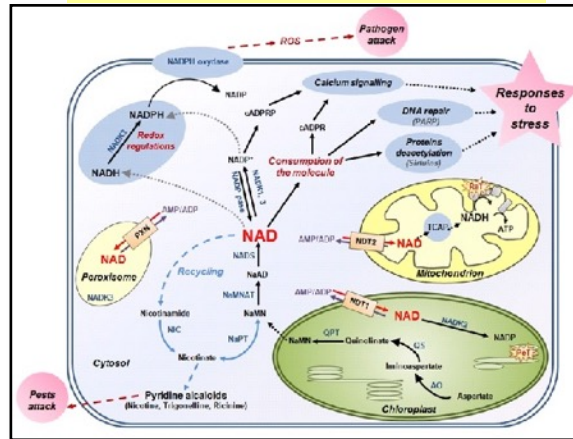


## Metabolomics profiles

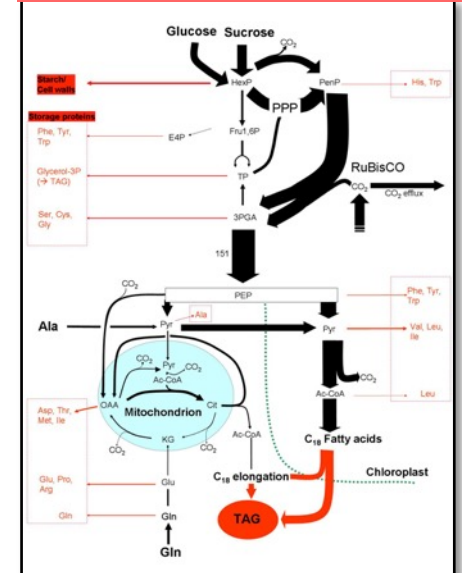
### Targeted or non targeted



## Biological system: Cell Metabolic pathway map



## Metabolic flux analysis



Car traffic



France = Road network



Car traffic



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

MERLION Metabolomics Workshop – 19-21<sup>th</sup> November 2014 – National University of Singapore





# RFMF Goals since 2005

## French Network for Metabolomics and Fluxomics

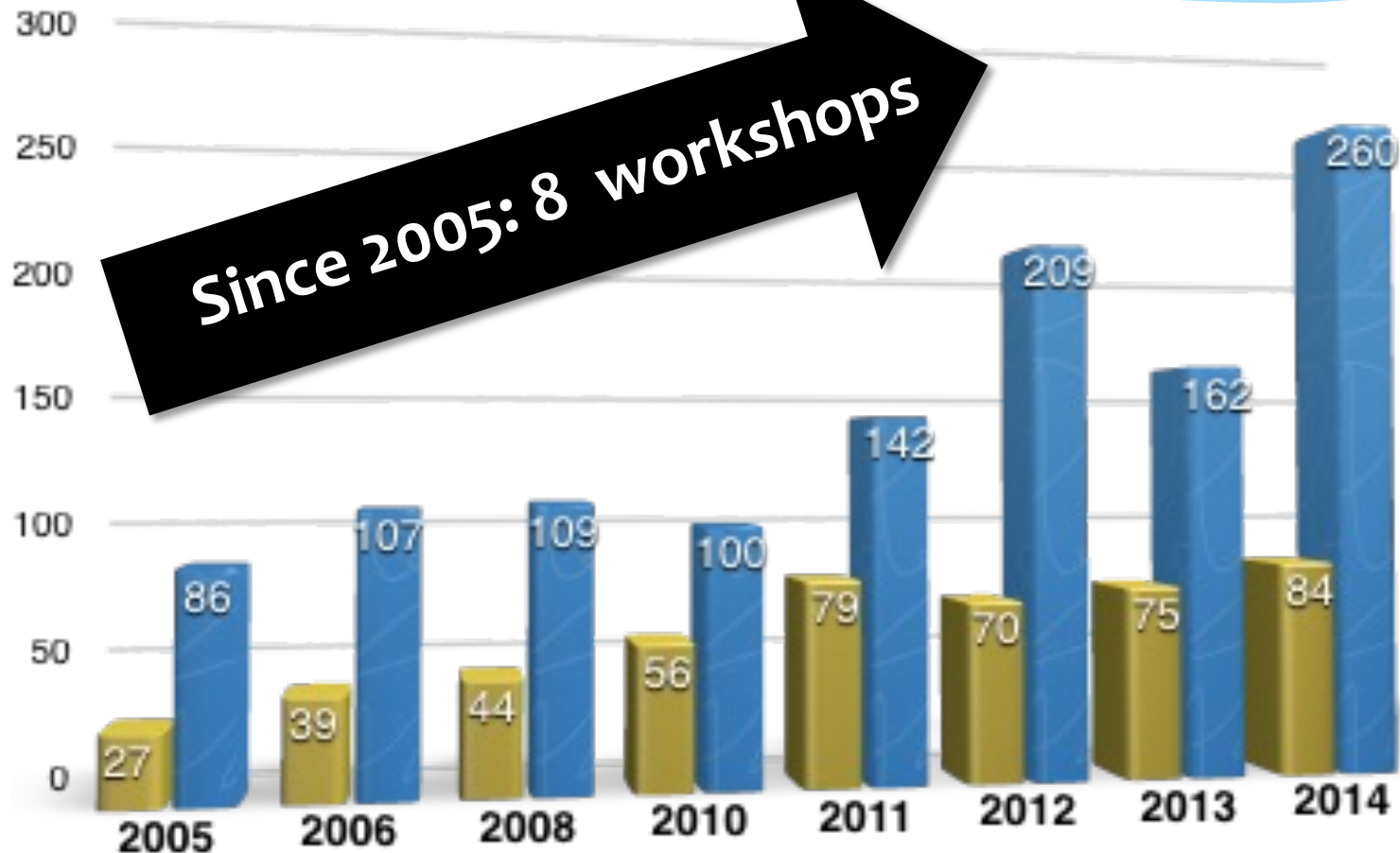
- Foster relationships between French researchers in M & F
- Promote and structure education and training in M & F
- Organize and support the organization of conferences in France
- Encourage through grants the participation of young researchers to national and international conferences
- Allocate funds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



RÉSEAU FRANÇAIS DE MÉTABOLOMIQUE ET FLUXOMIQUE

A growing community with a geographic & thematic expansion

■ Laboratoires & Entreprises ■ Participants



Since 2005: 8 workshops



-  Birmingham 1  
Cambridge 1  
Oxford 1  
Newcastle 2  
Dundee 1
-  Louvain 2  
Liège 1  
Kortrijk 1
-  Hanover 1
-  Genève 6
-  Sao Paulo 1
-  Naples 1  
Vicenza 1
-  Cluj-Napoca 1
-  Bratislava 1
-  Moncton 1

**260** Participants  
**84** French laboratories  
**16** Foreign laboratories



**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, softwares, procedures,



Next year in Lille



# 9 èmes Journées Scientifiques

# RFMF

RÉSEAU FRANÇAIS DE MÉTABOLOMIQUE ET FLUXOMIQUE

## June 2015 Villeneuve d'Ascq (Lille)



shop – 19-21<sup>th</sup> November 20

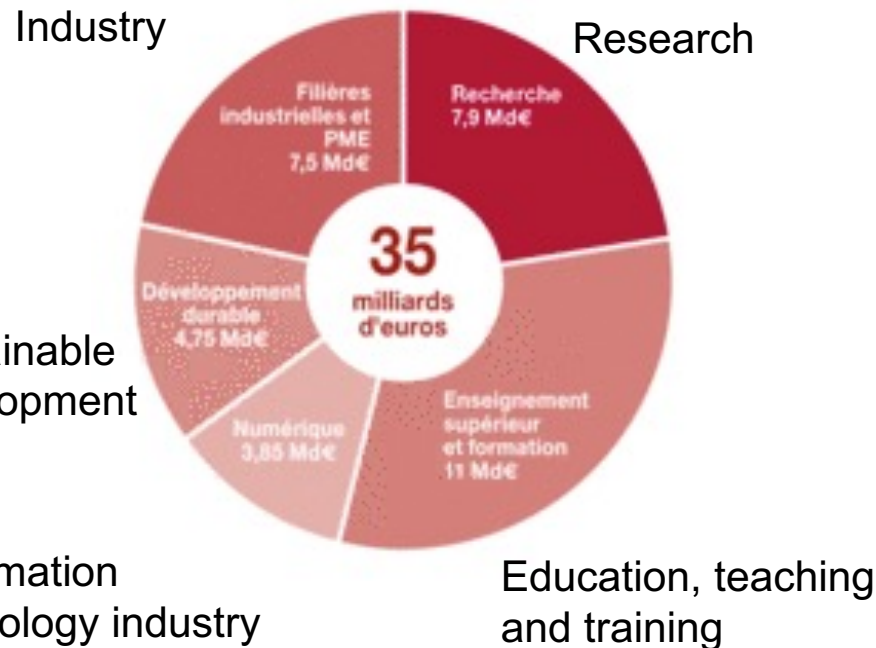


Metabo**HUB** is a French governmental “**top down**” initiative  
FRENCH STRATEGY FOR RESEARCH AND INNOVATION  
Investment Program for the Future (PIA) (2009)



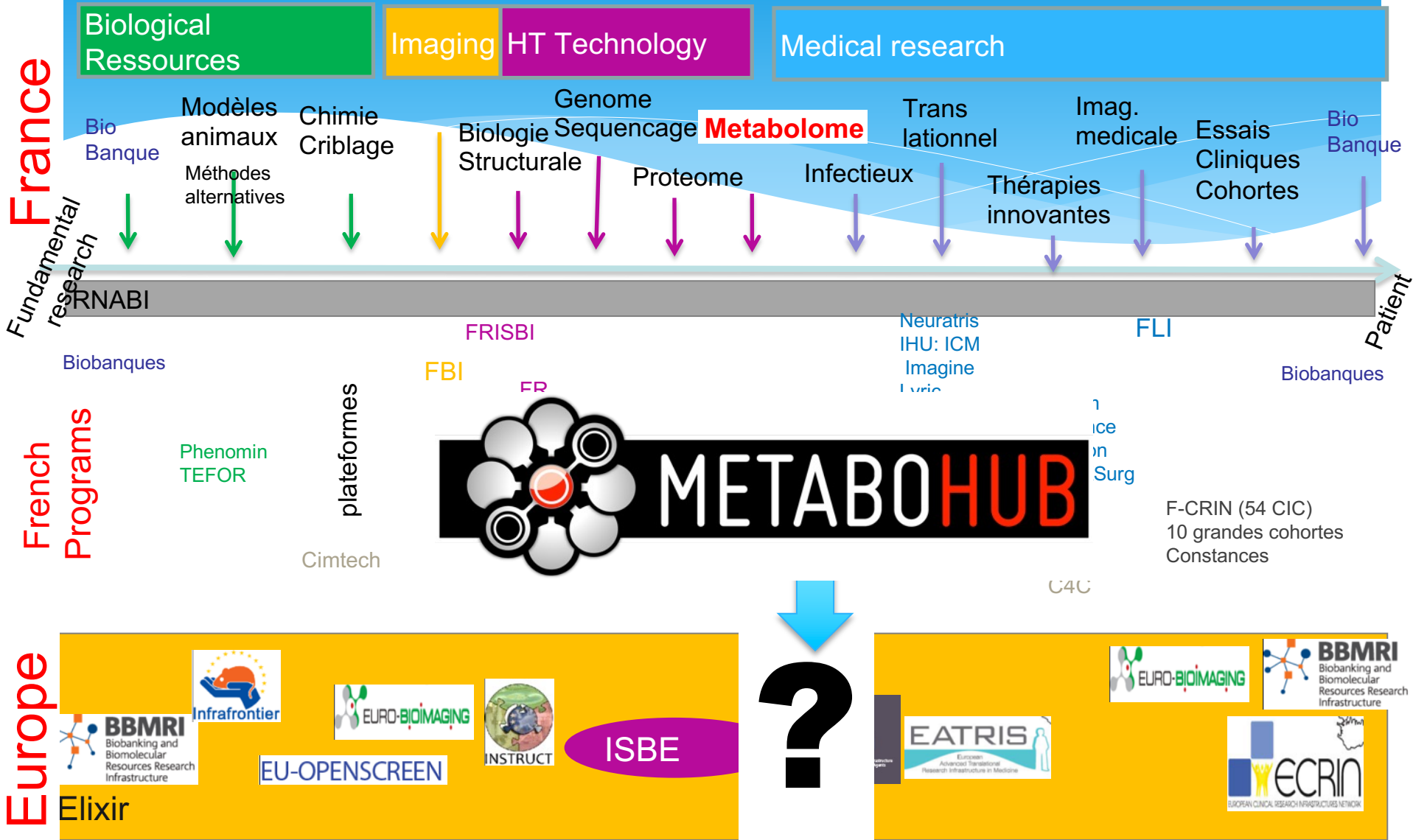
Selected areas (9)

- 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



# Global roadmap

## FRENCH STRATEGY FOR RESEARCH AND INNOVATION



03/07/2012

[catherine.chapel@recherche.gouv.fr](mailto:catherine.chapel@recherche.gouv.fr)

ESFRI= European Strategy Forum on Research Infrastructures



## 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 ...)

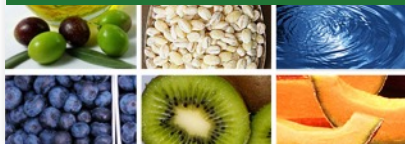
### **MetaboHUB strategy and Challenges**

Generic technology development in the core programme

Providing services to the french community

Technology translation in application projects in collaboration with associate partners

#### Food Science



#### Biotechnology



#### Environment



#### Human Health



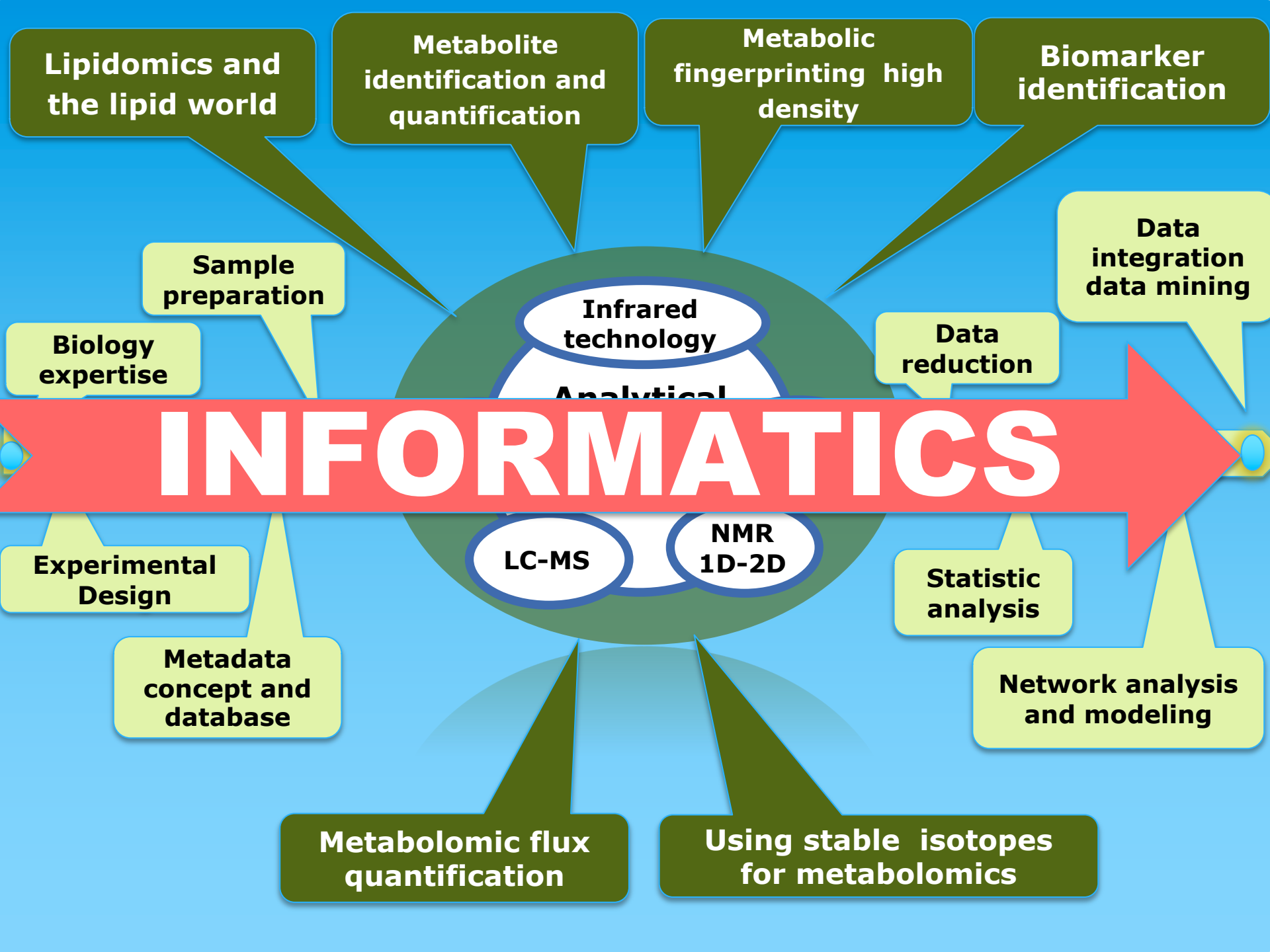


## Metabolomics and Fluxomics :

**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







## 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...

#### Human Health



#### Food Science



#### Biotechnology



#### Environment





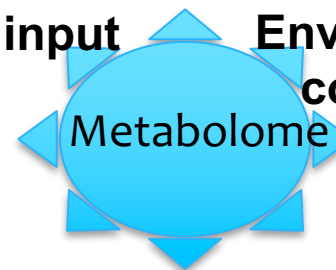
## Metabolomics is facing a world of complexity

### 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



## 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...



### 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

#### Human Health



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#### Food Science



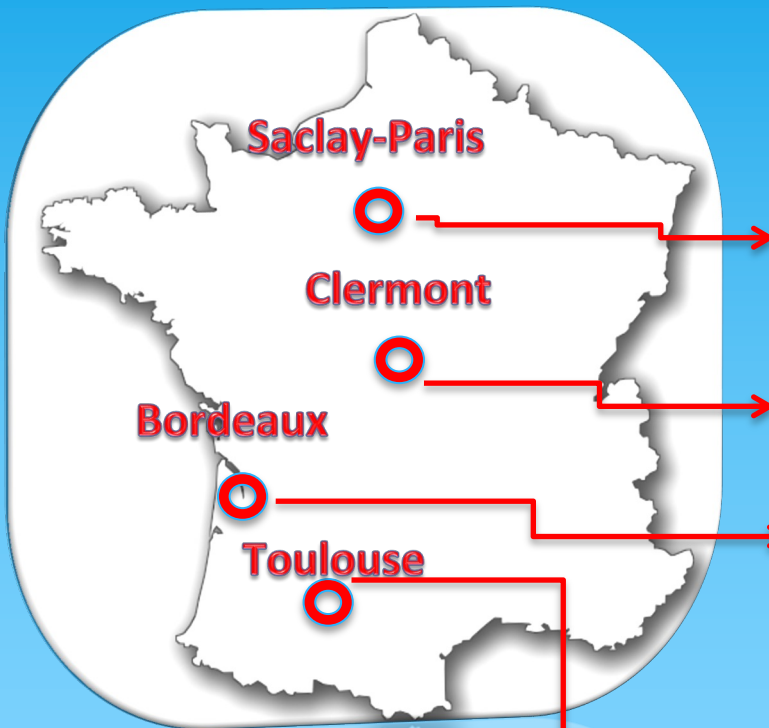
#### Biotechnology



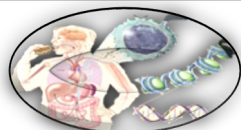
#### Environment



Bringing together 4 outstanding metabolomics platforms



Health & Clinical  
Microbiology  
**C. Junot**



Nutrition, Health  
& Environment  
**M. Ferrara**



Plant Biology &  
Biotechnology  
**A. Moing**




Microbiology,  
Biotechnology &  
Toxicology  
**JC Portais**




**7 NMR**


**NMR**



500 MHz

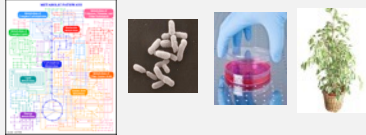


800 MHz



600 MHz

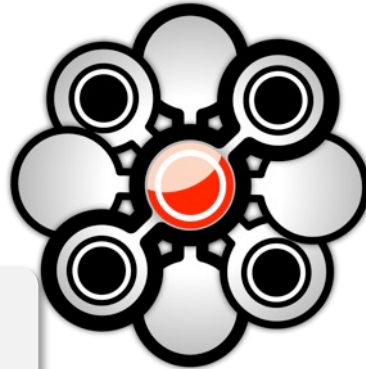
**Metabolic Flux (Bio)chemistry**



**Mass spectrometry**

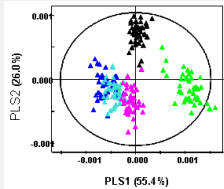


**27 LC MS  
11 GC MS**




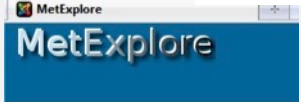
**8 servers  
2 data bases  
11 specialized software's**

**Bioinformatics, DB & Biomathematics**



PLS2 (26.0%)

PLS1 (55.4%)

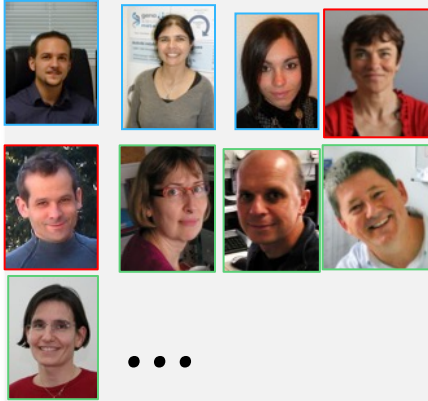
**Robotics & HT devices**



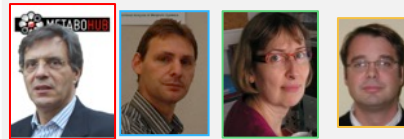
**5 Robots**



## NMR Expertise



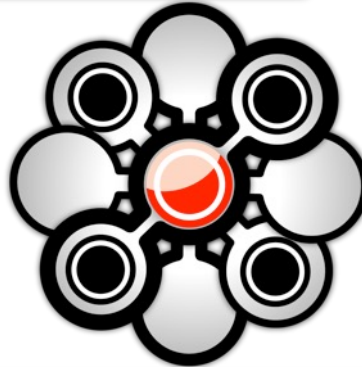
## Platform leaders



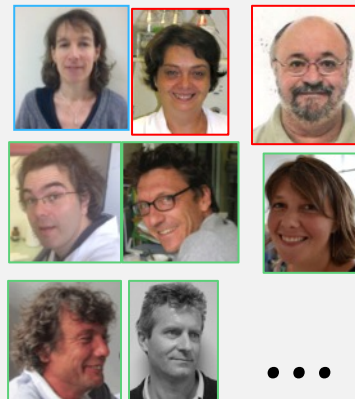
## MS Expertise



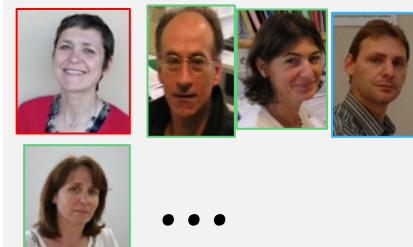
## Math & bioinfo Expertise



## Lipidomics Expertise



## Flux Expertise



Building term (2013-2016)  
Science & technological  
developments

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

**WP1 - Metabolomics**

**C. Junot**

**WP3 - Bioinformatics**

**E. Thevennot**

**WP2 - Fluxomics**

**JC. Portais**

**WP4 - Service**

**M. Ferrara**

**WP5 – Management  
WP6- Communication**

**C. Sautot**



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



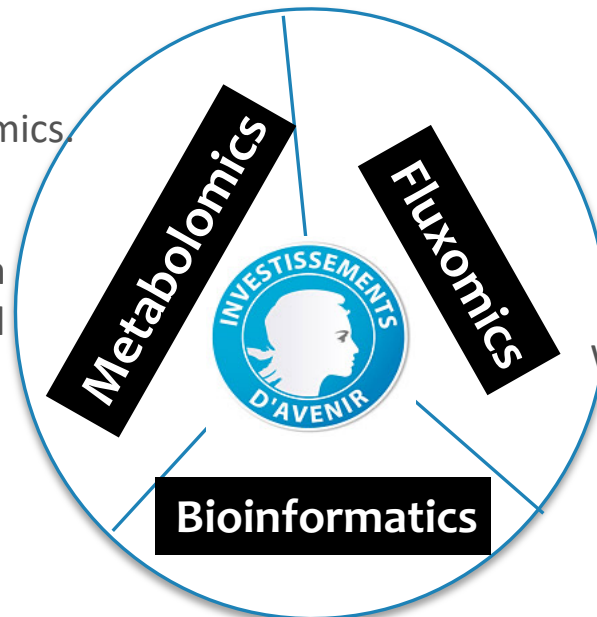
WP1b: Shared tools for lipidomics



WP1c: Tools for normalization and for quantitative MS-based metabolomics.



WP3: Shared bioinformatics tools for data management and data mining



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



WP2b: High-Throughput fluxomics



WP2c: Time and spatial resolution of the fluxome



**Human Health**



**Food Science**



**Biotechnology**



**Environment**





# Contribution of MetaboHUB to the MERLION Metabolomics Workshop

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



Non targeted metabolomics for assessment of environmental exposure to contaminant and their biological effects

Nutritional metabolomics as integrative understanding of metabolic disease development



9 NOV 2014 SINGAPOUR



Metabolic networking modelling and food Toxicity

Lipidomic analysis of palm oil variability

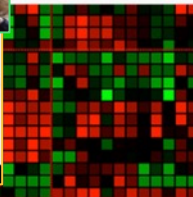


ON METABOLOMICS WOR  
SINGAPORE 2014



Application of metabolomic fingerprinting for food quality assessments

MS metabolomics and lipidomics for the study of rare diseases



MERLION METABOLOMICS WORKSHOP SINGAPORE

Developing Metabolomics Platform for Singapore-French Research  
Date: 19 - 21 November 2014  
Venue: University Town, National University of Singapore



A study on Honeybee losses: First insight into environmental interactions

Lipidomics: a key tool for human health



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

Biostatistic for biomarker discovery and phenotype prediction

Comprehensive investigations of cellular metabolic networks using 13C-fluxomics application to microbiology and biotechnology systems

Human Health

Food Science

Biotechnology

Environment



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Saclay

