



cgfb
CENTRE **BORDEAUX**
GÉNOMIQUE FONCTIONNELLE



cgfb

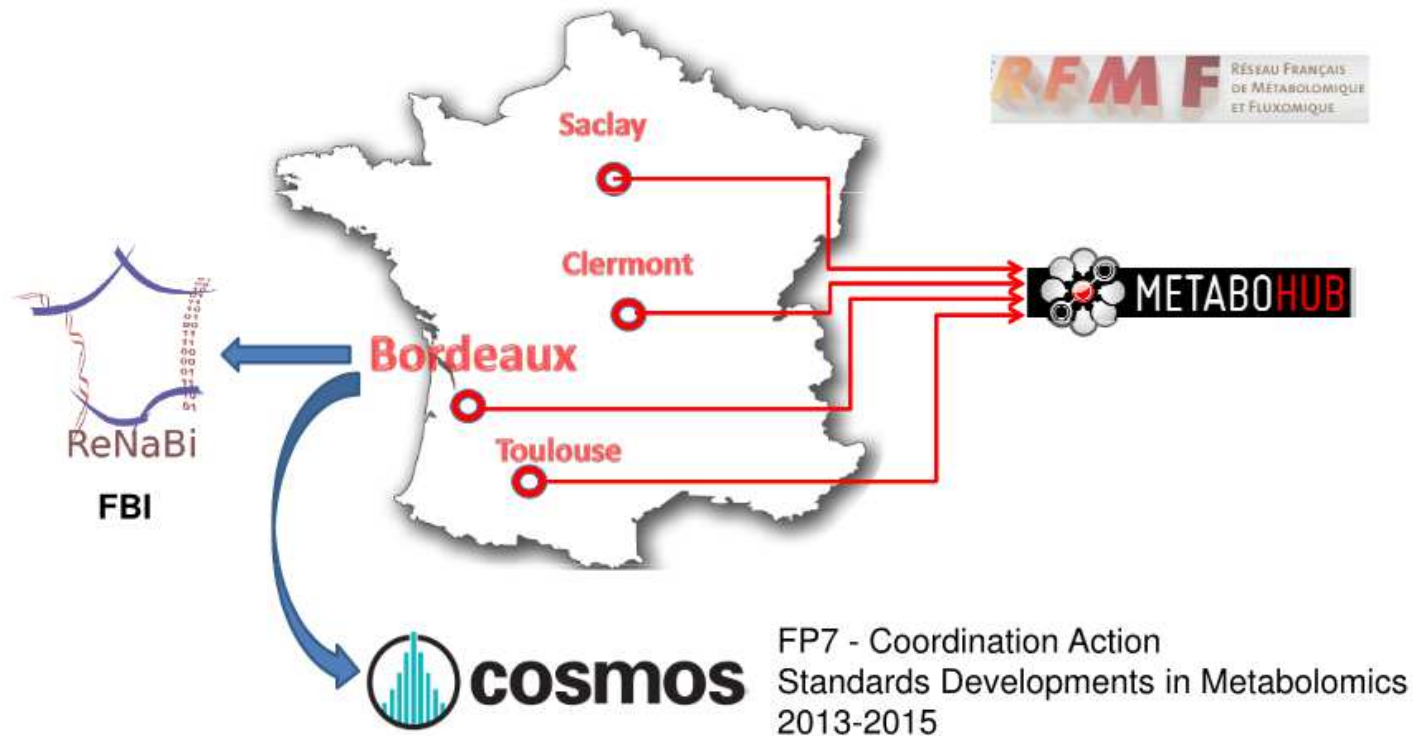
MÉTABOLOME

<http://www.cgfb.u-bordeaux2.fr/fr/metabolome>

La 1^{ère} PF Métabolome labellisée IBiSA
et PF Stratégique INRA 2008-2012

Annick Moing & Catherine Deborde

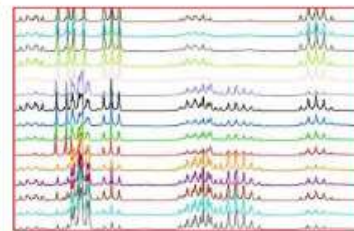
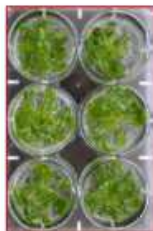
Networks



Bordeaux in the French metabolomics and bioinformatics infrastructures and networks

Fédérer des outils et savoir-faire pour l'étude du métabolisme

- **Satisfaire les besoins en métabolomique non ciblée ou ciblée et phénotypage métabolique haut débit liés aux activités de recherche** de laboratoires académiques et privés
 - **services ou collaboration**
 - identification et/ou analyse de métabolites (LC, RMN et MS),
 - mesure d'enrichissements isotopiques après marquage ^{13}C
- **Ouverture** à l'ensemble de la communauté pour la mise à disposition de services, d'équipements et d'expertise
- **Formation**, Ecole Chercheur
- **Accueil** de masters, doctorants, chercheurs



- **Métabolome – Lipidome – Profils & Phénotypage métaboliques**

0. Métadonnées échantillons

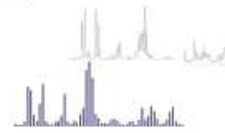
1. Extraction(s)



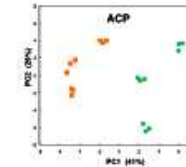
**2. Analyses biochimiques
ciblées ou non**



3. Pré-traitement des données



4. Visualisation et exploration des données



5. Intégration des données

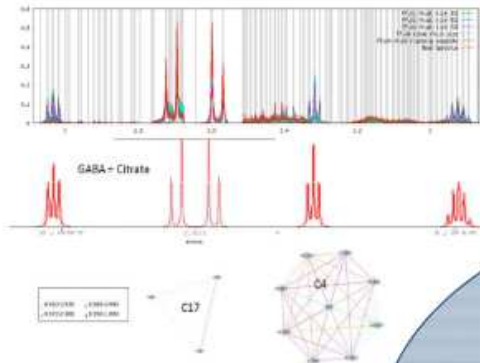


Bioinformatic Activities



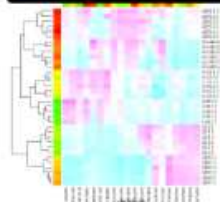
MeRY-B is a plant metabolomics knowledgebase allowing the storage and visualisation of metabolic profiles.

Ferry-Dumazet et al. BMC Plant Biology



Data Management	
1)	Brassica oleracea var. Italica (1)
8)	Cucumis melo (8)
1)	Elaeis guineensis (1)
1)	Fragaria x ananassa (1)
14)	Lycopersicon esculentum (14)
2)	Medicago truncatula
1)	Oryza sativa (1)
1)	Ostreococcus lauri (1)
1)	Phoenix dactylifera (1)
1)	Prunus persica (1)
1)	Vanilla planifolia (1)
2)	Vitis vinifera (2)
2)	Zea mays (2)

Spectra Processing & Data mining



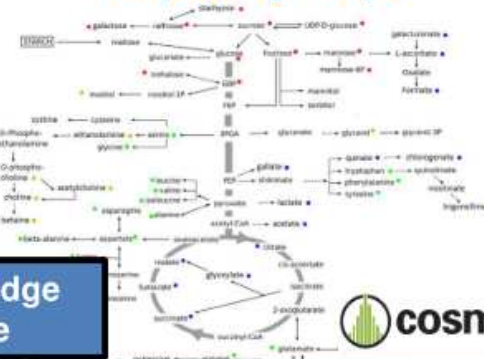
Data Analysis

<http://bit.ly/biostatflow>

BioStatFlow

Knowledge Base

<http://bit.ly/meryb>

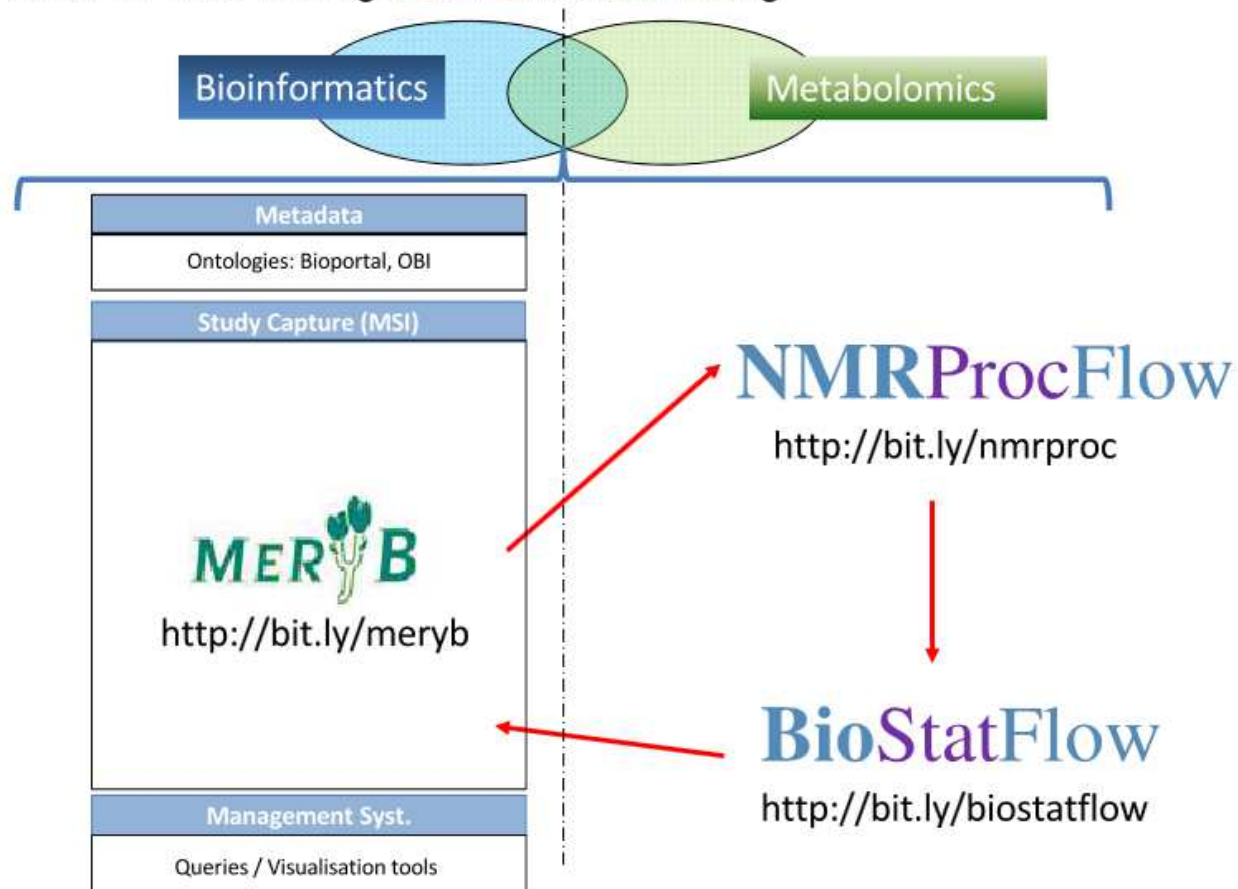


Open Data (COSMOS-compliant)

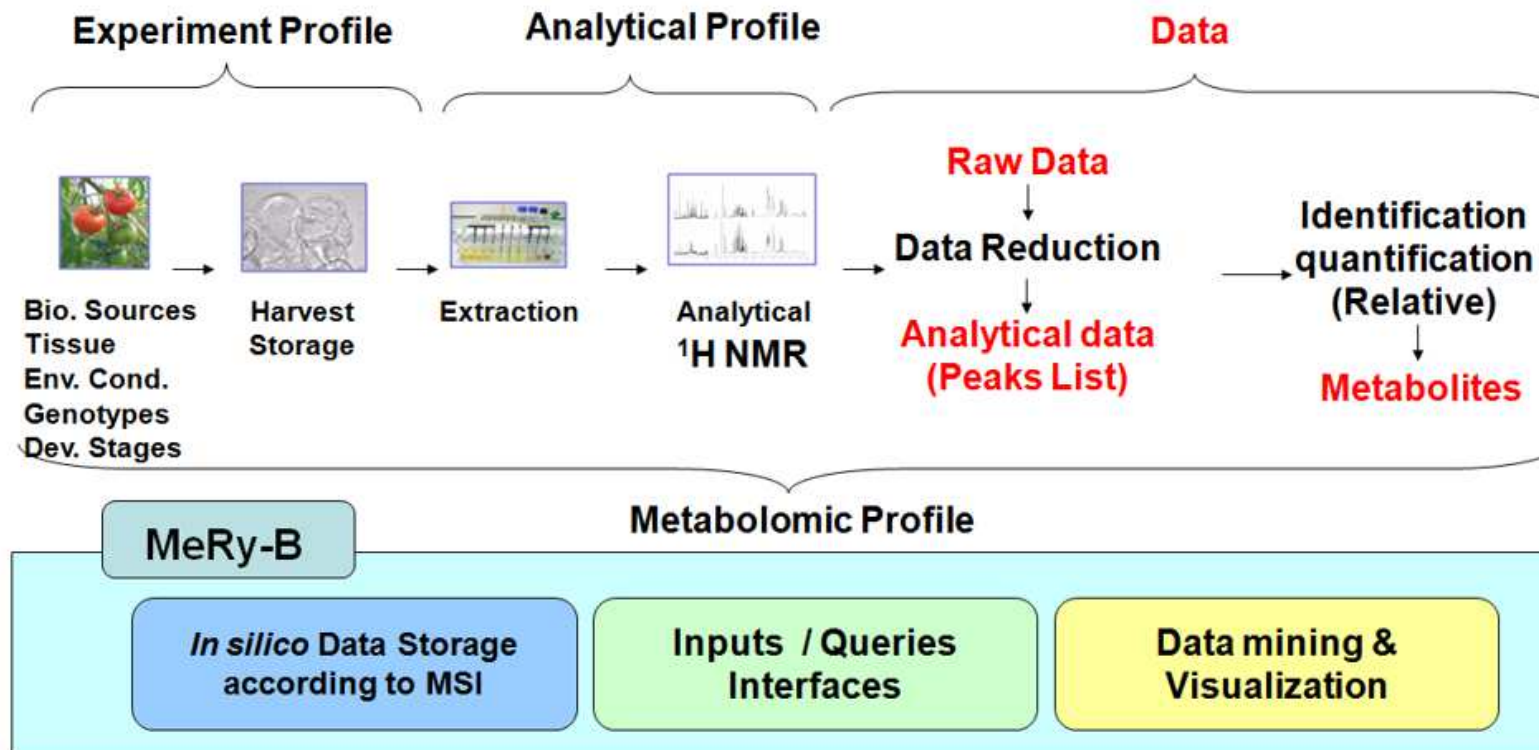
Metabolomics & Bioinformatics



- **Design and Implementation :**
 - Tools for data management and data mining



Strategy





<http://www.cbib.u-bordeaux2.fr/MERYB/>

Metabolomic Repository Bordeaux

MeRy-B is a plant metabolomics knowledgebase allowing the storage and visualisation of metabolic profiles from plants ... [read more](#)

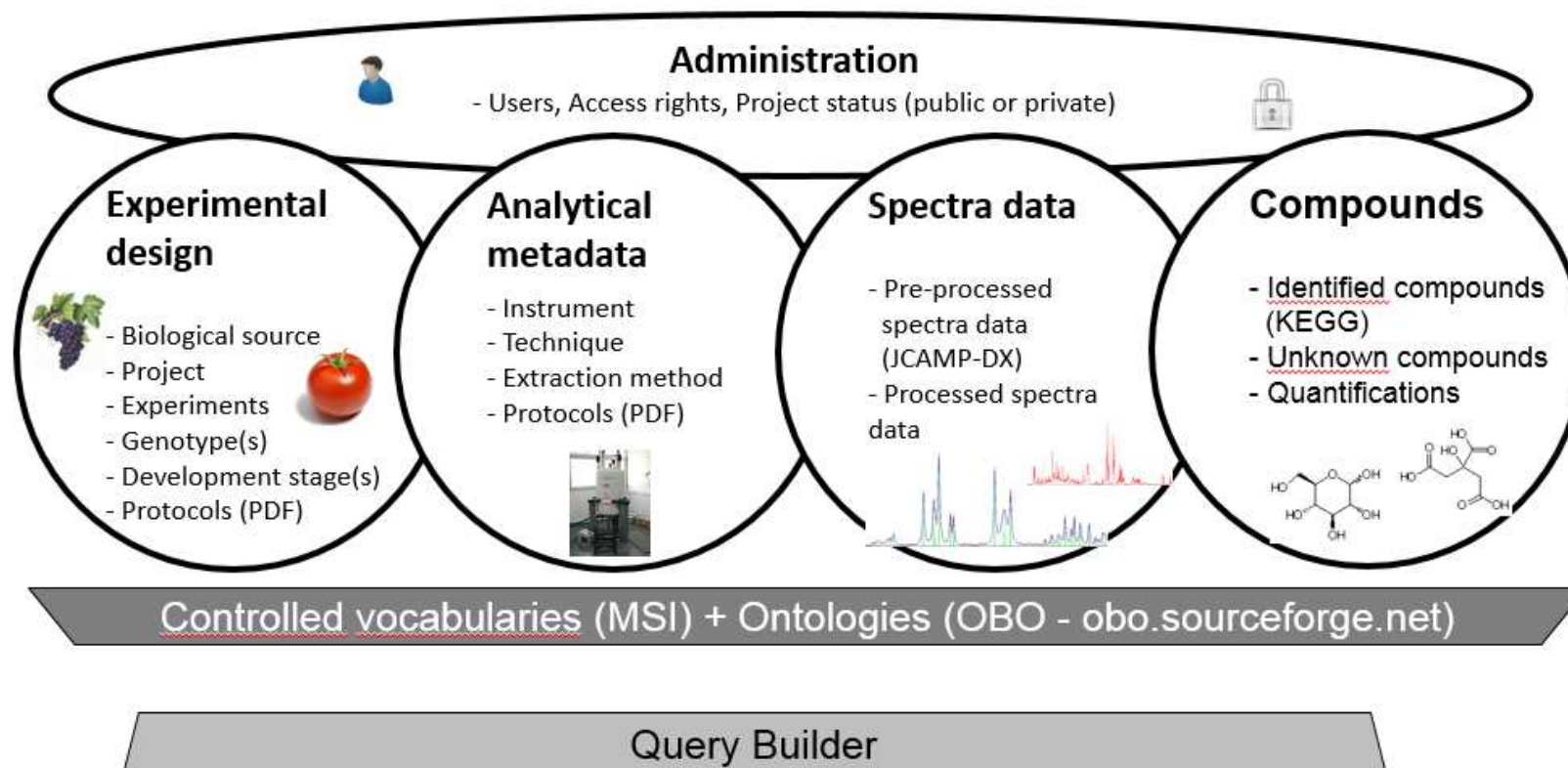
Summary (public/all)

Projects :	17 / 41	(41%)
Experiments :	42 / 107	(39%)
Plants :	199 / 464	(43%)
Spectra :	1027 / 2063	(50%)
Compounds :	138 / 180	(77%)



MSI-Compliant & OBO-Compliant

Ferry-Dumazet H., Jacob D *et al* BMC Plant Biology 2011



Tomato- Metabolomics - 2006 (T06002) | Lycopersicon esculentum
UMR 619 Biologie du Fruit - INRA, University Bordeaux 1 and 2 - Bordeaux (France)

Description
Global approach to characterize changes in metabolic profiles in two interdependent tissues Seed and Flesh from the same tomato fruits during tomato fruit development.

Reference: DOI:10.1007/s11306-007-0059-1
Fabien Moumet, Martine Lemaire-Chamley, Mickaël Maucourt, Cécile Cabasson, Jean-Luc Giraudel, Catherine Deborde, René Lessire, Philippe Gallucci, Anne Bertrand, Monique Gaudillère, Christophe Rothan, Dominique Rolin and Annick Moing. Quantitative metabolic profiles of tomato flesh and seeds during fruit development: complementary analysis with ANN and PCA. *Metabolomics*, 2007, 3:273-288

Select:

Experiment Name	Tissue/Organ	Env. Conditions	BS	GT	I	Dev. Stage	Tech	SD
Tomato-Seed	seed	Normal	WT	Ailsa Craig	1	FF.01 fruit size 30% (8) FF.02 fruit size 50% (12) FF.03 fruit size 70% (20) FF.04 final fruit size (35) FR.04 fruit ripening complete (45)	1H NMR	25
Tomato-Flesh	fruit	Normal	WT	Ailsa Craig	1	FF.01 fruit size 30% (8) FF.02 fruit size 50% (12) FF.03 fruit size 70% (20) FF.04 final fruit size (35) FR.04 fruit ripening complete (45)	1H NMR	29

Legends:

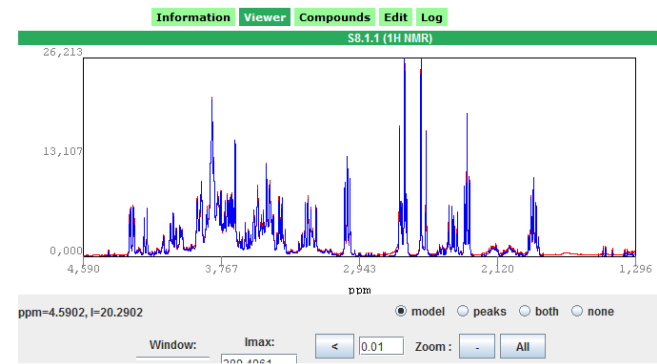
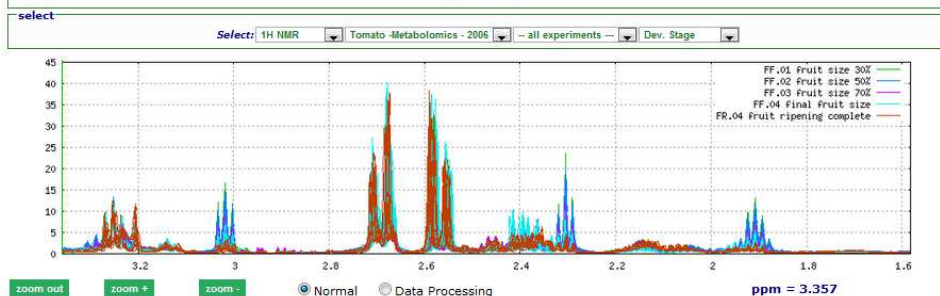
Env. Conditions	Environmental Conditions	Dev. Stage	Development Stage
BS	Background	Tech	Analytical technique
GT	Genotype	SD	Number of Spectral Data
I	Number of Individuals		

Tissue/Organ	Environmental Conditions	Study Type
seed	Normal	growth chamber study

Growth Protocol		Harvest Protocol				Storage Protocol
PG-Tomato - Metabolomics - 2006		PH-Tomato - Metabolomics - 2006				PS-Tomato-UMR619-1

Background	Genotype - Ind Code	FF.01 fruit size 30%	FF.02 fruit size 50%	FF.03 fruit size 70%	FF.04 final fruit size	FR.04 fruit ripening complete
WT	Ailsa Craig : Seed	S8.1.1 - 1H NMR	S12.1.1 - 1H NMR	S20.1.1 - 1H NMR	S35.1.1 - 1H NMR	S45.1.2 - 1H NMR
		S8.2.1 - 1H NMR	S12.2.1 - 1H NMR	S20.2.1 - 1H NMR	S35.2.1 - 1H NMR	S45.2.2 - 1H NMR
		S8.3.1 - 1H NMR	S12.3.1 - 1H NMR	S20.3.1 - 1H NMR	S35.3.1 - 1H NMR	S45.3.2 - 1H NMR
		S8.123.2 - 1H NMR	S12.3.2 - 1H NMR	S20.3.2 - 1H NMR	S35.3.2 - 1H NMR	

Lycopersicon esculentum
Tomato- Metabolomics - 2006
Global approach to characterize changes in metabolic profiles in two interdependent tissues Seed and Flesh from the same tomato fruits during tomato fruit development.



Nb	Name	User synonym	Shift/Multiplicity	Comment	Quantification	Links
1	4-Aminobutanoate	GABA	1.92 m 2.3 t	C3H2 C2H2	- 33925.2 µg/g DW	MRB7
2	5-Oxoproline	pyroglutamic acid	4.18 dd	C4H2	-	MRB21
3	Acetylcholine	Acetylcholine	3.22 s	N-(C(5)H3)3	-	MRB5
4	Alanine	Alanine	1.48 d	C(3)H3	497.819 µg/g DW	MRB53
5	Asparagine	Asparagine	2.92 m	C(3)H2	1810.78 µg/g DW	MRB35
6	Aspartate	Aspartate	2.81 m	1/2(C(3)H2)	1098.79 µg/g DW	MRB56
7	Chlorogenate	chlorogenic acid	6.4 d 6.96 d 7.13 d 7.21 d 7.68 d	Caffeoyl-C8H Caffeoyl-C7H	- 7195.01 µg/g DW	MRB11
8	Choline	Choline	3.2 s	N-(C(3)H3)3	1262.99 µg/g DW	MRB6
9	Citrate	Citrate	2.63 dd	C(2)H2+ C(4)H2	38088.1 µg/g DW	MRB12
10	D-Galactose	galactose	4.6 d	β C(1)H	-	MRB79
11	D-Mannose	Mannose	5.2 d	C(1)H	41.9992 µg/g DW	MRB44
12	Formate	Formate	8.47 s	C(1)H	-	MRB15
13	Fructose	Fructose	4.12 m	alphaC(3)H+ C(5)H+alphaC(5)H	17603.1 µg/g DW	MRB14
14	Fumarate	fumaric acid	6.53 s	C(2)H+ C(3)H	87.7298 µg/g DW	MRB15
15	Glucose	Glucose	4.66 d 5.25 d	β-C1H alpha-C1H	- 48123.6 µg/g DW	MRD45
16	Glutamate	Glutamate	2.07 m	C(3)H2	16784.7 µg/g DW	MRB17
17	Glutamine	Glutamine	2.45 m	C(4)H2	3842.45 µg/g DW	MRB18
18	Isoleucine	Isoleucine	1.01 d	C(6)H3	90.6444 µg/g DW	MRB39
19	L-Threonine	Threonine	1.33 d	C(4)H3	124.392 µg/g DW	MRB90
20	Leucine	Leucine	0.96 t	C(5)H3+ C(6)H3	419.67 µg/g DW	MRB100
21	Malate	Malate	4.3 dd	C(2)H	23451.4 µg/g DW	MRB19
22	II-Methylnicotinate	Trigonelline	4.44 s 8.08 t 8.83 m 9.13 s	C(3)H	- 311.49 µg/g DW	MRB23
23	Phenylalanine	Phenylalanine	7.4 m	C(5)H+ C(6)H+ C(7)H	638.754 µg/g DW	MRB20
24	Sucrose	Sucrose	5.41 d	Glucopyranosyl-C(1)H	30806.9 µg/g DW	MRB22
25	Tyrosine	Tyrosine	6.91 d	C(6)H2	212.941 µg/g DW	MRB25
26	UDP-glucose	UDPG	5.98 m		410.142 µg/g DW	MRB102
27	Valine	Valine	1.04 d	C(5)H3	305.852 µg/g DW	MRB92
28	unkD5.1	UnknownD5.1	5.1 d		-	MRB159
29	unkD6.2	Adenosine-like	6.2 d	C1H of ribose	200.558 µg/g DW	MRB101
30	unkD7.55	UnknownD7.55	7.55 d	Caffeoyl-CxH	-	MRB160
31	unkS5.4	UnknownS5.4	5.4 s		86.1868 µg/g DW	MRB104
32	unkS5.55	UnknownS5.55	5.55 s		66.0024 µg/g DW	MRB161
33	unkS8.5	UnknownS8.5	8.5 s		131.229 µg/g DW	MRB106



S8.1.1 (1H NMR)						
Nb	Name	User synonym	Shift/Multiplicity	Comment	Quantification	Links
1	4-Aminobutanoate	GABA	1.92 m	C3H2	-	MRB7
			2.3 t	C2H2	-	
			3.01 t	C4H2	33925.2 µg/g DW	
2	5-Oxoproline	pyroglutamic acid	4.18 dd	C2H	-	MRB21
3	Acetylcholine	Acetylcholine	3.22 s	N-(C(5)H3)3	-	MRB5
4	Alanine	Alanine	1.48 d	C(3)H3	497.819 µg/g DW	MRB63
5	Asparagine	Asparagine	2.92 m	C(3)H2	1810.78 µg/g DW	MRB85
6	Aspartate	Aspartate	2.81 m	1/2(C(3)H2)	1098.79 µg/g DW	MRB96
7	Chlorogenate	chlorogenic acid	6.4 d	Caffeoyl-C8H	-	MRB11
			6.96 d	-	-	
			7.13 d	-	-	
			7.21 d	-	-	
			7.68 d	Caffeoyl-C7H	7195.01 µg/g DW	
8	Choline	Choline	3.2 s	N-(C(3)H3)3	1262.99 µg/g DW	MRB6
9	Citrate	Citrate	2.63 dd	C(2)H2+ C(4)H2	38088.1 µg/g DW	MRB12
10	D-Galactose	galactose	4.6 d	β C(1)H	-	MRB79
11	D-Mannose	Mannose	5.2 d	C(1)H	41.9992 µg/g DW	MRB44
12	Formate	Formate	8.47 s	C(1)H	-	MRB13
13	Fructose	Fructose	4.12 m	alphaC(3)H+ C(5)H+alphaC(5)H	17603.1 µg/g DW	MRB14
14	Fumarate	fumaric acid	6.53 s	C(2)H+ C(3)H	87.7298 µg/g DW	MRB15
15	Glucose	Glucose	4.66 d	β-C1H	-	MRB45
			5.25 d	alpha-C1H	48123.6 µg/g DW	
16	Glutamate	Glutamate	2.07 m	C(3)H2	16784.7 µg/g DW	MRB17
17	Glutamine	Glutamine	2.45 m	C(4)H2	3842.45 µg/g DW	MRB18
18	Isoleucine	Isoleucine	1.01 d	C(6)H3	90.6444 µg/g DW	MRB89
19	L-Threonine	Threonine	1.33 d	C(4)H3	124.392 µg/g DW	MRB90
20	Leucine	Leucine	0.96 t	C(5)H3+ C(6)H3	419.67 µg/g DW	MRB100
21	Malate	Malate	4.3 dd	C(2)H	23451.4 µg/g DW	MRB19
22	N-Methylnicotinate	Trigonelline	4.44 s	-	-	MRB23
			8.08 t	-	-	
			8.83 m	-	-	
			9.13 s	C(3)H	311.49 µg/g DW	
23	Phenylalanine	Phenylalanine	7.4 m	C(5)H+ C(6)H+ C(7)H	638.754 µg/g DW	MRB20
24	Sucrose	Sucrose	5.41 d	Glucopyranosyl-C(1)H	30806.9 µg/g DW	MRB22
25	Tyrosine	Tyrosine	6.91 d	C(6)H2	212.941 µg/g DW	MRB25
26	UDP-glucose	UDPG	5.98 m	-	410.142 µg/g DW	MRB102
27	Valine	Valine	1.04 d	C(5)H3	305.852 µg/g DW	MRB92
28	unkD5.1	UnknownD5.1	5.1 d	-	-	MRB159
29	unkD6.2	Adenosine-like	6.2 d	C1H of ribose	200.558 µg/g DW	MRB101
30	unkD7.55	UnknownD7.55	7.55 d	Caffeoyl-CxH	-	MRB160
31	unkS5.4	UnknownS5.4	5.4 s	-	86.1868 µg/g DW	MRB104
32	unkS5.55	UnknownS5.55	5.55 s	-	66.0024 µg/g DW	MRB161
33	unkS8.5	UnknownS8.5	8.5 s	-	131.229 µg/g DW	MRB106



MeRy-B Card
ID: MRB7

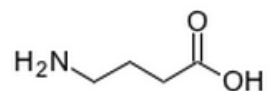
Name	4-Aminobutanoate	Summary	
User synonym	GABA	Species	9
CTD	3889297	Tissue/Organ	10
HMDB ID	HMDB00112	Analytical Technique	1

- C00334
- MRB7 Others Links
- MRB7 Pathways & Reactome
- HMDB00112 NMR Peak List
- MRB7 1H NMR Quantification Peak List
- MRB7 NMR Spectrum

Filters

Species	Tissue/Organ	Technique	Sort
-----	-----	-----	Species

Species	Arabidopsis thaliana	Project name	Arabidopsis thaliana hydrophilic metabolome	
Tissue/Organ	cultured cell	Experiment name	Methanol/Chloroform/Water extraction	
1H NMR Shifts	2.301:t	No quantification		
Species	Cucumis melo	Project name	Charentais Melon Fruit 2008 - Anal Chem 2009	
Tissue/Organ	fruit	Experiment name	1-Major metabolites of melon flesh	
1H NMR Shifts	3.02:t	Min: 0.26 mg/g DW	Max: 1.22 mg/g DW	
Species	Cucumis melo	Project name	Charentais Melon Fruit 2009- Spatial 2- META-PHOR	
Tissue/Organ	fruit	Experiment name	Escrito - Slice 2	
1H NMR Shifts	3.02:t	Min: 534.793 µg/g DW	Max: 1266.14 µg/g DW	
Species	Cucumis melo	Project name	Charentais Melon Fruit 2009- Spatial 2- META-PHOR	
Tissue/Organ	fruit	Experiment name	Escrito - Slice 3	
1H NMR Shifts	3.02:t	Min: 1098.44 µg/g DW	Max: 1407.44 µg/g DW	
Species	Elaeis guineensis mesocarp	Project name	Palm tree 2011	
Tissue/Organ	mesocarp	Experiment name	Palm tree	
1H NMR Shifts	1.92:m	No quantification		
Species	Lycopersicon esculentum	Project name	Tomato Leaf & long-term cadmium stress - 2010	
Tissue/Organ	leaf	Experiment name	Leaf 100 microM	
1H NMR Shifts	3.02:t	Min: 724.942 µg/g DW	Max: 1141.21 µg/g DW	
Species	Lycopersicon esculentum	Project name	Tomato Leaf & long-term cadmium stress - 2010	
Tissue/Organ	leaf	Experiment name	Leaf 100 microM	
1H NMR Shifts	3.02:t	Min: 724.942 µg/g DW	Max: 1141.21 µg/g DW	



C00334

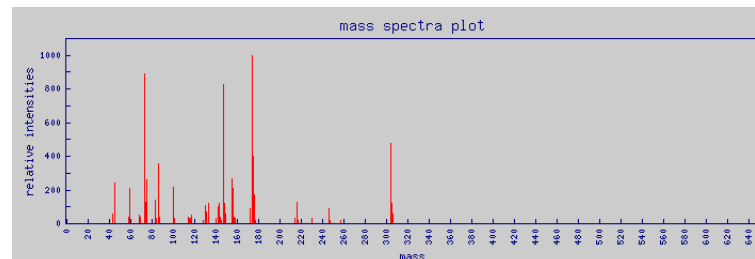
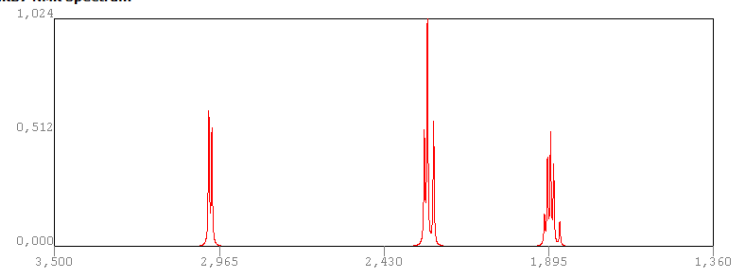
Chemical entities of biological interest

- 1 amino acid
- 1 biphenyl carboxylic acid
- 1 carbohydrate acid
- 1 cefalotin
- 1 cefditoren
- 1 cefpiramide
- 1 cefpodoxime
- 1 cefpodoxime proxetil
- 1 chlorocarboxylic acid
- 1 cinalukast
- 1 clofibric acid
- 1 dicarboxylic acid
- 1 gibberellin
- 1 hexacarboxylic acid
- 1 hydroxy carboxylic acid
- 1 indolyl carboxylic acid
- 1 monocarboxylic acid
- 1 naptalam
- 1 octacarboxylic acid
- 1 oxo carboxylic acid
- 1 penicillanic acids
- 1 penillic acid
- 1 pentacarboxylic acid
- 1 phosphonoformic acid
- 1 poly(methacrylic acid) macromolecule
- 1 steroid acid
- 1 sulfur-containing carboxylic acid
- 1 tetracarboxylic acid
- 1 treprostinil
- 1 tricarboxylic acid
- 1 ureidocarboxylic acid
- 1 verteporfin

Biological Pathways

- 4-aminobutyrate degradation IV
- IAA biosynthesis I
- IAA biosynthesis II
- alanine biosynthesis II
- alanine biosynthesis III
- alanine degradation II (to D-lactate)
- alanine degradation III
- beta-alanine biosynthesis II
- biotin biosynthesis II
- gamma-coniciene and coniine biosynthesis
- glutamate degradation IV
- hypoglycin biosynthesis
- indole-3-acetyl-amino acid biosynthesis
- lupanine biosynthesis
- molybdenum cofactor biosynthesis
- phenylalanine degradation III
- serinol biosynthesis
- tRNA charging pathway

MRB7 NMR Spectrum





Resource-based approach



- Access to resources separately and directly => URL nomenclature
- URLs : <http://www.cbib.u-bordeaux2.fr/MERYB/res/<resource>/<ID>/<option>>
- URI scheme : [meryb:resource:identifiant](http://www.cbib.u-bordeaux2.fr/MERYB/res/<resource>/<ID>/<option>)

Tomato- Metabolomics - 2006 (T06002) | Lycopersicon esculentum
UMR 619 Biologie du Fruit - INRA, University Bordeaux 1 and 2 - Bordeaux (France)

Description
Global approach to characterize changes in metabolic profiles in two interdependent tissues Seed and Flesh from the same tomato fruits during tomato fruit development.

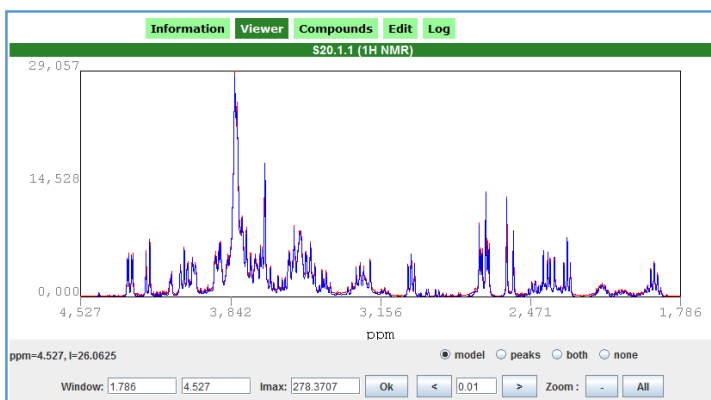
Reference: DOI:10.1007/s11306-007-0059-1

Fabien Mounet, Martine Lemaire-Chamley, Mickaël Maucourt, Cécile Cabasson, Jean-Luc Giraudel, Catherine Deborde, René Lessire, Philippe Gallucci, Anne Bertrand, Monique Gaudillère, Christophe Rothlan, Dominique Rollin and Annick Moing. Quantitative metabolic profiles of tomato flesh and seeds during fruit development: complementary analysis with ANR and PCA. *Metabolomics*, 2007, 3:272-280

select
Select: -- all experiments --

Experiment Name	Tissue/Organ	Env. Conditions	BS	GT	I	Dev. Stage	Tech	SD
Tomato-Seed	seed	Normal	WT	Ailsa Craig	1	FF.01 fruit size 30% (8) FF.02 fruit size 50% (12) FF.03 fruit size 70% (20) FF.04 final fruit size (35) FR.04 fruit ripening complete (45)	1H NMR	25
Tomato-Flesh	fruit	Normal	WT	Ailsa Craig	1	FF.01 fruit size 30% (8) FF.02 fruit size 50% (12) FF.03 fruit size 70% (20) FF.04 final fruit size (35) FR.04 fruit ripening complete (45)	1H NMR	29

<http://www.cbib.u-bordeaux2.fr/MERYB/res/project/T06002>



<http://www.cbib.u-bordeaux2.fr/MERYB/res/spectra/S20.1.1>

MeRy-B Card
ID: MRB7

Name	4-Aminobutanoate	Summary
User synonyms	GABA	Species: 9
CTS	3889297	Tissue/Organ: 10
HMDB ID	HMDB00112	Analytical Technique: 1

C00334
 MRB7 Others Links

CHEBI: CHEBI:16865 KNAPSACK: C00001337 MPIMP: 153003 PLANTCYC: 4-AMINO-BUTYRATE

MRB7 Pathways & Reactome
Expand: all | none

- 4-aminobutyrate degradation I
 - 2-ketoglutarate + 4-aminobutyrate -> L-glutamate + succinate semialdehyde 2.6.1.19
- 4-aminobutyrate degradation IV
 - 4-aminobutyrate + pyruvate = succinate semialdehyde + L-alanine 2.6.1.19
- glutamate degradation IV
 - 2-ketoglutarate + 4-aminobutyrate -> L-glutamate + succinate semialdehyde 2.6.1.19
 - 4-aminobutyrate + pyruvate = succinate semialdehyde + L-alanine 2.6.1.19
 - L-glutamate + H+ -> CO2 + 4-aminobutyrate 4.1.1.15
- putrescine degradation IV
 - 4-aminobutanal + NAD+ + H2O -> 4-aminobutyrate + NADH + 2 H+ 1.2.1.19

HMDB00112 NMR Peak List
 MRB7 1H NMR Quantification Peak List
 MRB7 NMR Spectrum

ppm=2.965, I=1.024

<http://www.cbib.u-bordeaux2.fr/MERYB/res/compound/MRB7>



Resource-based approach



- Access to resources separately and directly => URL nomenclature
- URLs : <http://www.cbib.u-bordeaux2.fr/MERYB/res/<resource>/<ID>/<option>>
- URI scheme : `meryb:resource:identifiant`

Tomato 2006

MeRy-B Project | Spectra Overlay | Bucket Analysis | Metabolite Analysis

Tomato- Metabolomics - 2006 (T06002) | *Lycopersicon esculentum*
UMR 619 Biologie du Fruit - INRA, University Bordeaux 1 and 2 - Bordeaux (France)

Description
Global approach to characterize changes in metabolic profiles in two interdependent tissues: Seed and Flesh from the same tomato fruits during tomato fruit development

Reference: DOI:10.1007/s11306-007-0059-1

Fabien Mounet, Martine Lemaire-Chamley, Mickaël Maucourt, Cécile Cabasson, Jean-Luc Giraud, Annick Moing. Quantitative metabolic profiles of tomato flesh and seeds during fruit development

Select

Experiment Name	Tissue/Organ	Env. Conditions
Tomato-Flesh	pericarp	Normal
Tomato-Seed	seed	Normal

Scaling

- normalization_QQ_KDE
- normalization_boxplot

PCA

- PCA_summary
- PCA-scores_1-2
- PCA-scores_1-3
- PCA_pclar

One-way ANOVA

- anova_FaCl
- anova_FaCl

HCA

- ColHCA
- HeatMap
- RowHCA

bswfllog

- All results

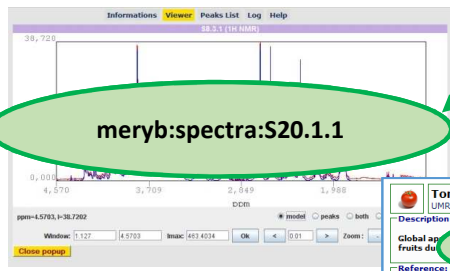
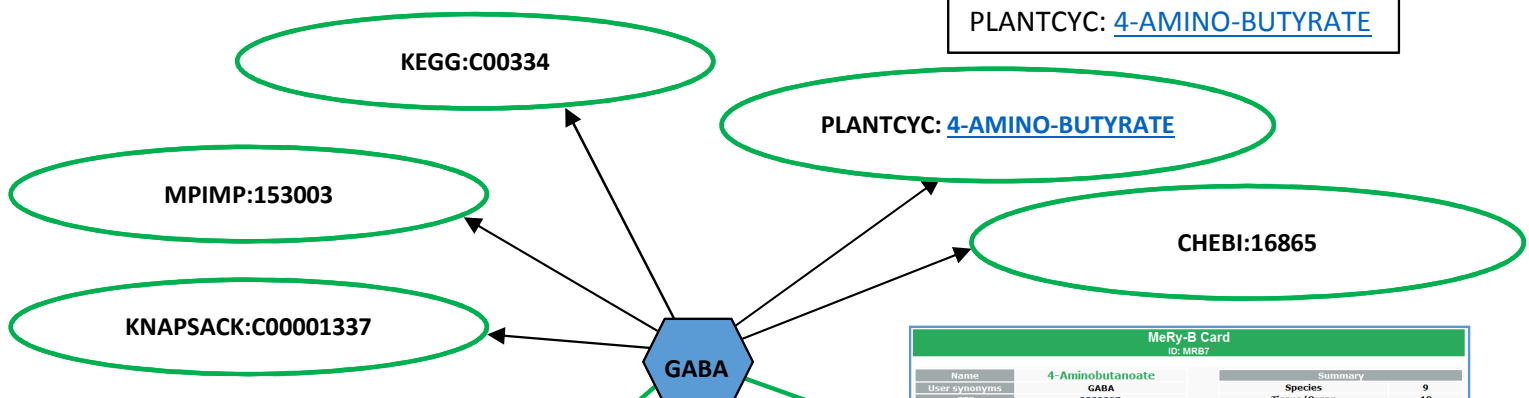
p6/anova_FaCl.png Zoom: + - Download

Mashup approach
(ROA/REST; *Web 2.0*)

Resource-based approach

Extension of the links network ...

MERYB Compound
 Name : GABA
 KEGG: [C00334](#)
 CHEBI : [16865](#)
 KNAPSACK: [C00001337](#)
 MPIMP: [153003](#)
 PLANTCYC: [4-AMINO-BUTYRATE](#)



MeRy-B Card
 ID: MRB7

Name	4-Aminobutanoate	Summary
User Synonyms	GABA	Species
CIS	3889297	Tissue/Organ
HMDB ID	HMDB00112	Analytical Technique

meryb:compound:MRB7 4-AMINO-BUTYRATE

MRB7 Pathway

- Expand: all | none
- 4-aminobutyrate degradation IV
 - 2-ketoglutarate + 4-aminobutyrate -> L-glutamate + succinate semialdehyde 2.6.1.19
- 4-aminobutyrate degradation IV
 - 4-aminobutyrate + pyruvate = succinate semialdehyde + L-alanine 2.6.1.19
- glutamate degradation IV
 - 2-ketoglutarate + 4-aminobutyrate -> L-glutamate + succinate semialdehyde 2.6.1.19
 - 4-aminobutyrate + pyruvate = succinate semialdehyde + L-alanine 2.6.1.19
 - glutamate + H+ -> CO2 + 4-aminobutyrate 4.1.1.15
- IV
 - anal + NAD+ + H2O -> 4-aminobutyrate + NADH + 2 H+ 1.2.1.19

Peak List

Tomato - Metabolomics - 2006 (T06002) | Lycopersicon esculentum
 UMR 619 Biologie du Fruit

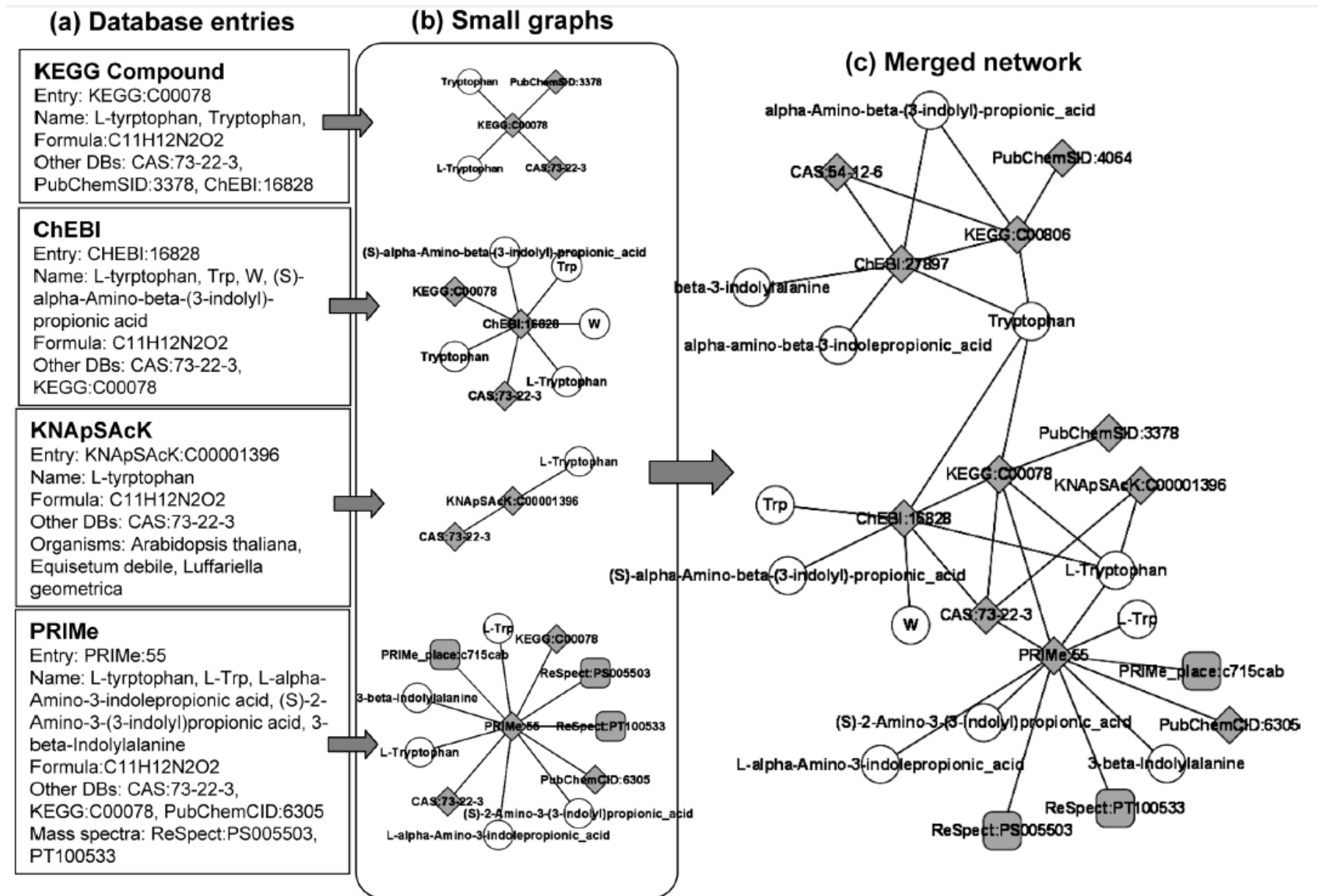
Description
 Global app fruits du

References
 Fabien Mounet, Martine Lemaire-Chabry, ...

select
 Select: -- all experiments --

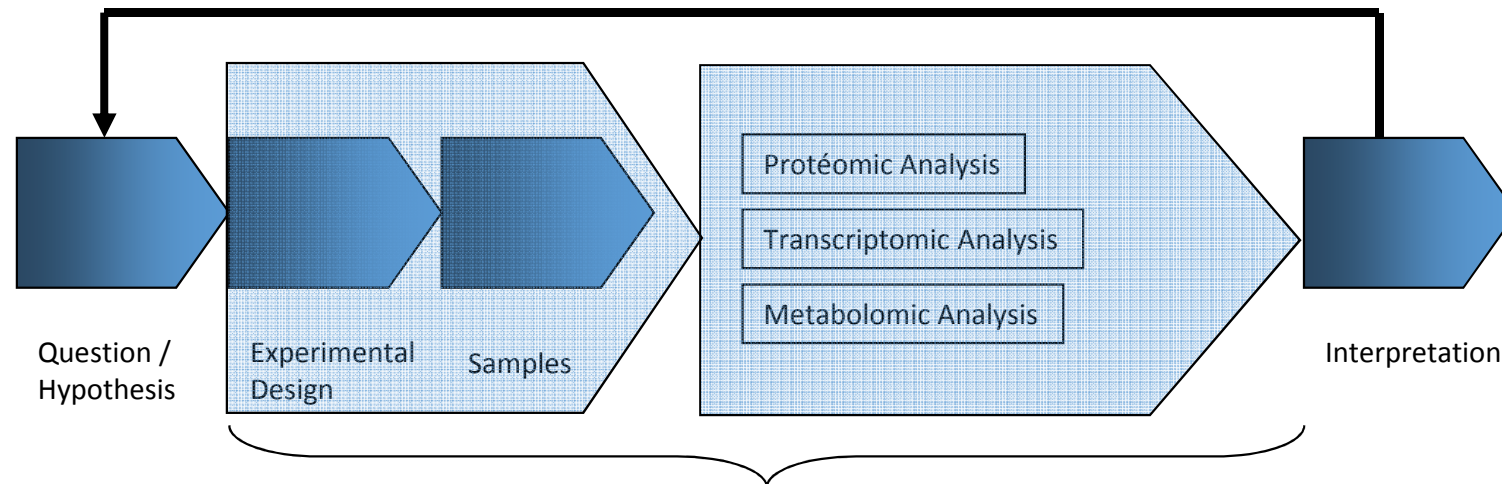
Experiment Name	Tissue/Organ	Env. Conditions	BS	GT	I	Dev. Stage	Tech	SD
Tomato-Seed	seed	Normal	WT	Ailsa Craig	1	FF.01 fruit size 30% (8) FF.02 fruit size 50% (12) FF.03 fruit size 70% (20) FF.04 final fruit size (25) FR.04 fruit ripening complete (45)	1H NMR	25
Tomato-Flesh	fruit	Normal	WT	Ailsa Craig	1	FF.01 fruit size 30% (8) FF.02 fruit size 50% (12) FF.03 fruit size 70% (20) FF.04 final fruit size (25) FR.04 fruit ripening complete (45)	1H NMR	28





Data commoning

Integrative Biology



biosharing

Partners, Locations
(QA & QC)

STANDARDS

formats terminologies checklists

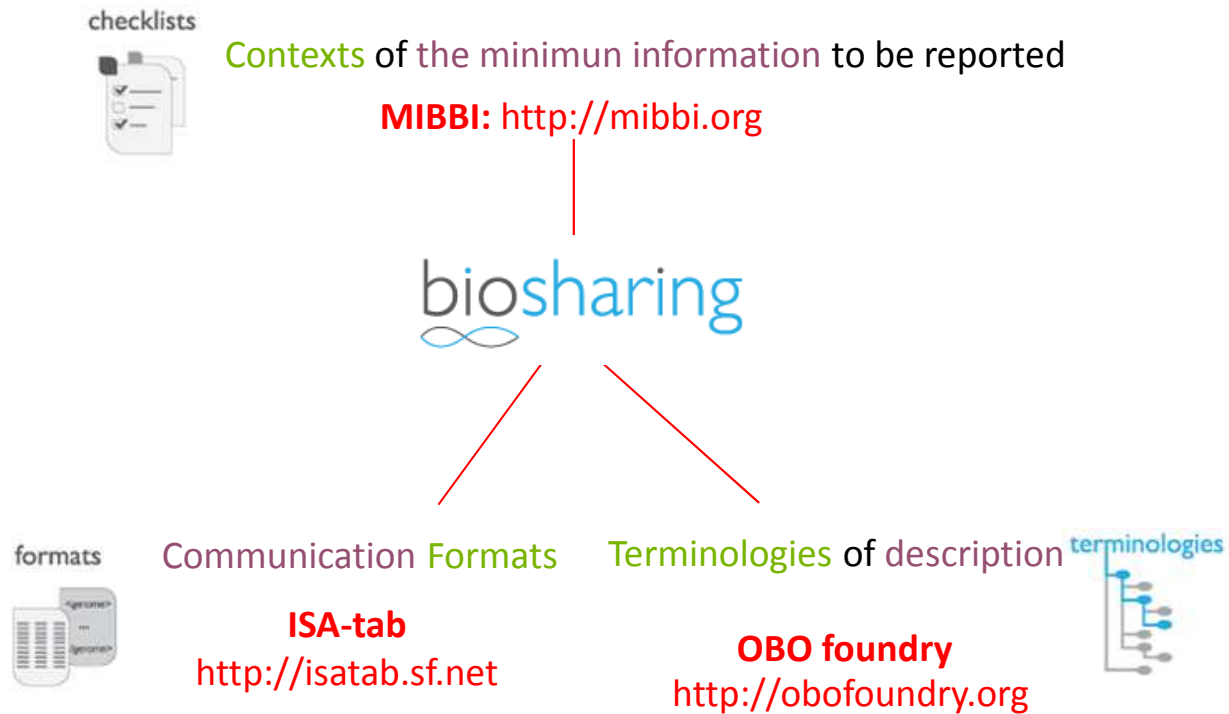


- Link data in the context of metadata
- Positive and lasting impact on the value of scientific results

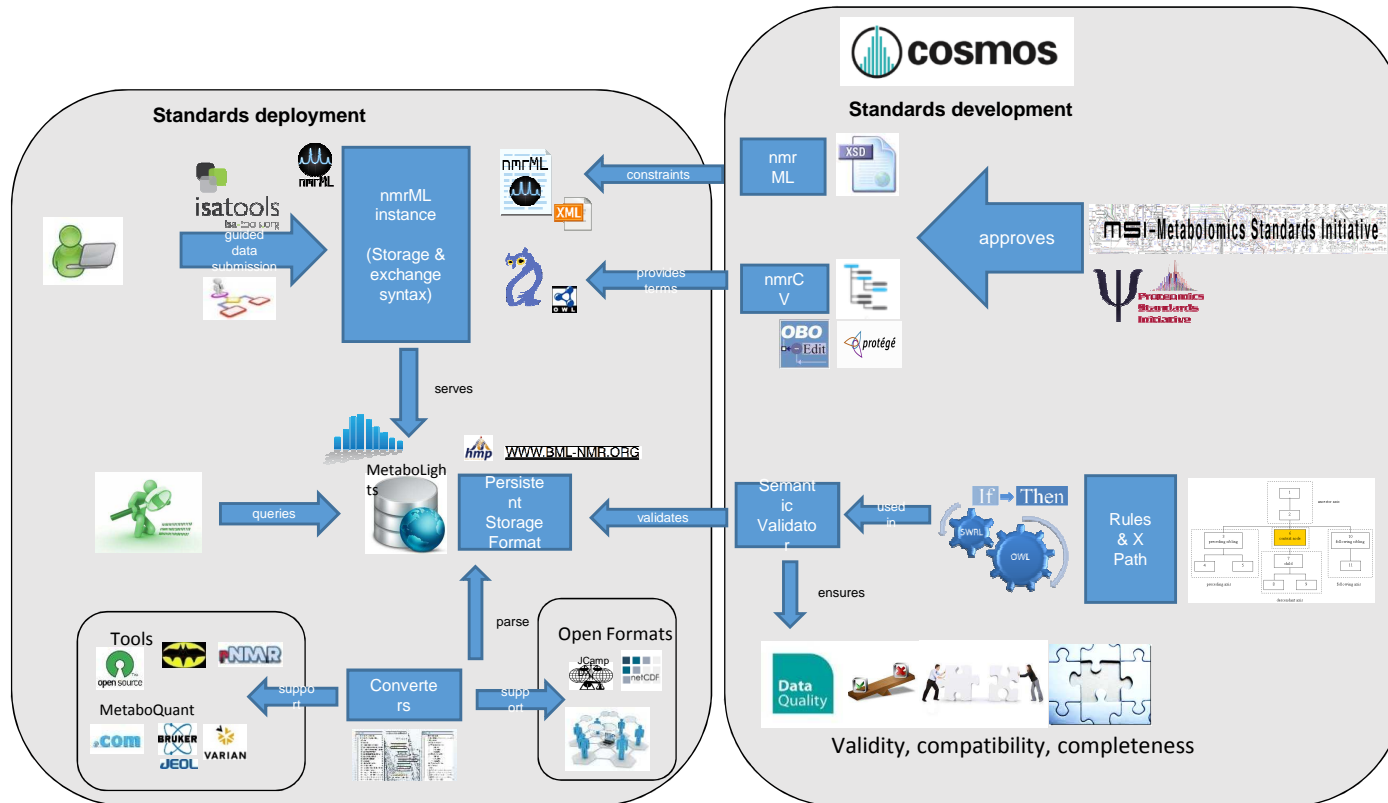
A catalogue of reporting standards (minimum reporting guidelines, exchange formats and terminologies) and organizations that develop these.

Data commoning

→ Ensure consistency between the metadata



COSMOS data annotation, verification, and distribution workflow

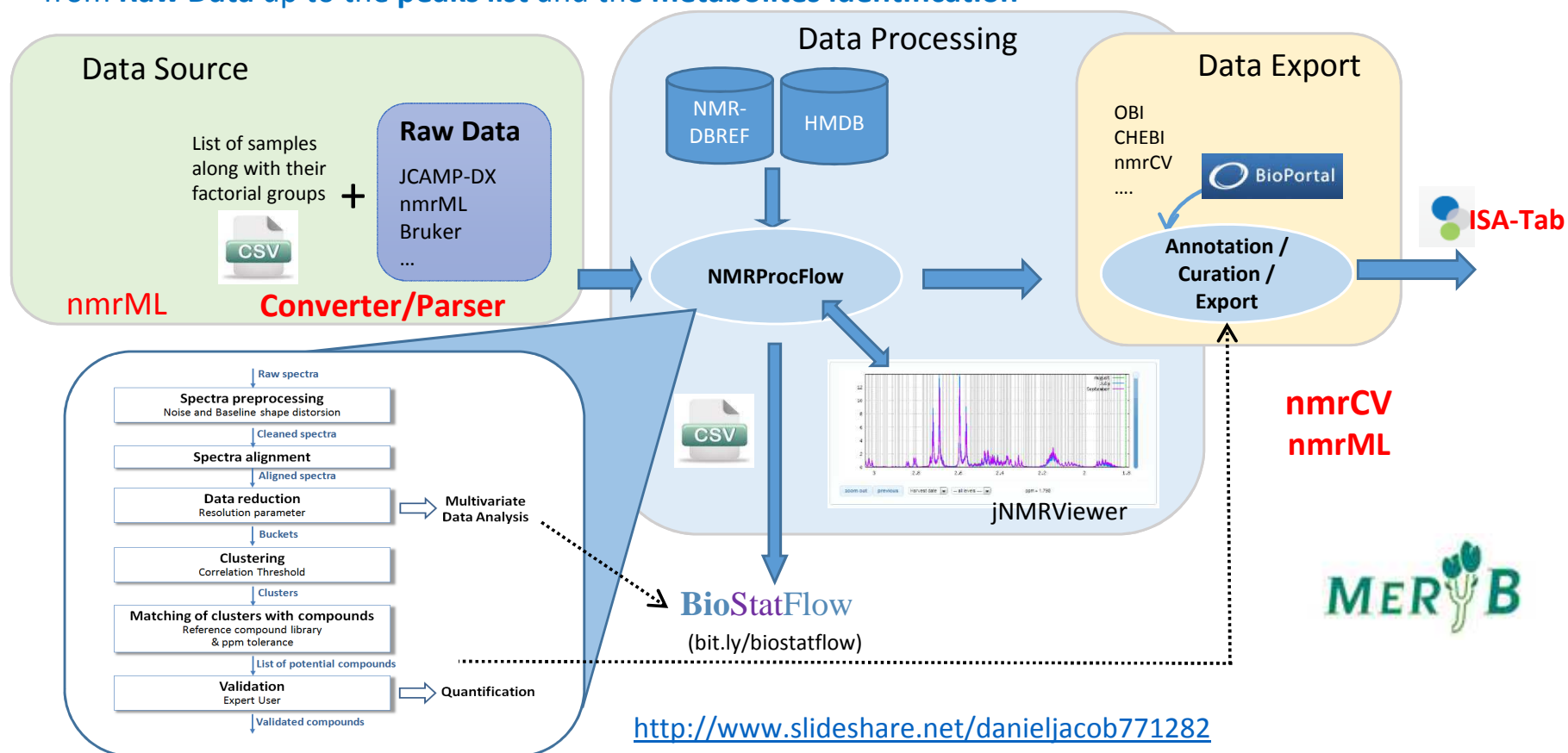


nmrML

nmrCV

Converter/Parser

An efficient spectra processing **workflow** for metabolite identification from ^1H -NMR metabolomics data from **Raw Data** up to the **peaks list** and the **metabolites identification**



Jacob D. *et al*, (March 2013) Analytical and Bioanalytical Chemistry. DOI:10.1007/s00216-013-6852-y

Remerciements :

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PMFB

Stéphane Bernillon

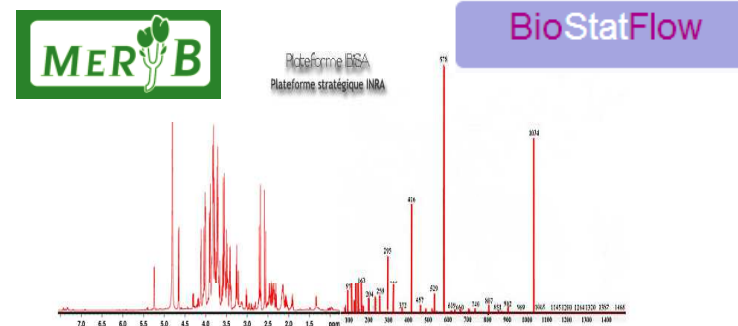
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Mickaël Maucourt

Annick Moing

Dominique Rolin



<http://bit.ly/meryb>

<http://bit.ly/biostatflow>

<https://code.google.com/p/nmr-viewer/>

