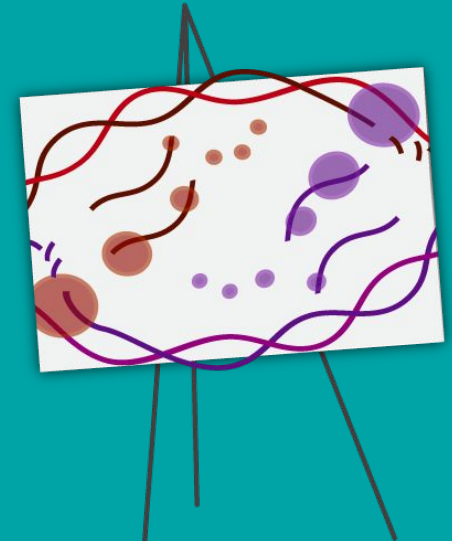


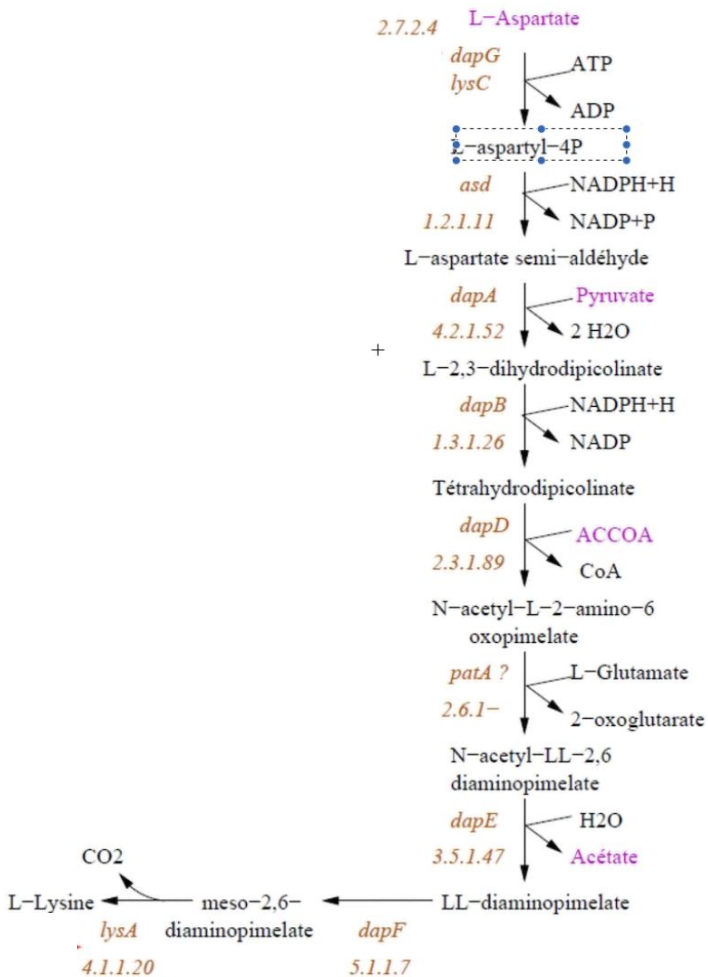
INRAE

> Présentation d'Escher -- Outil de visualisation de données dans un réseau métabolique

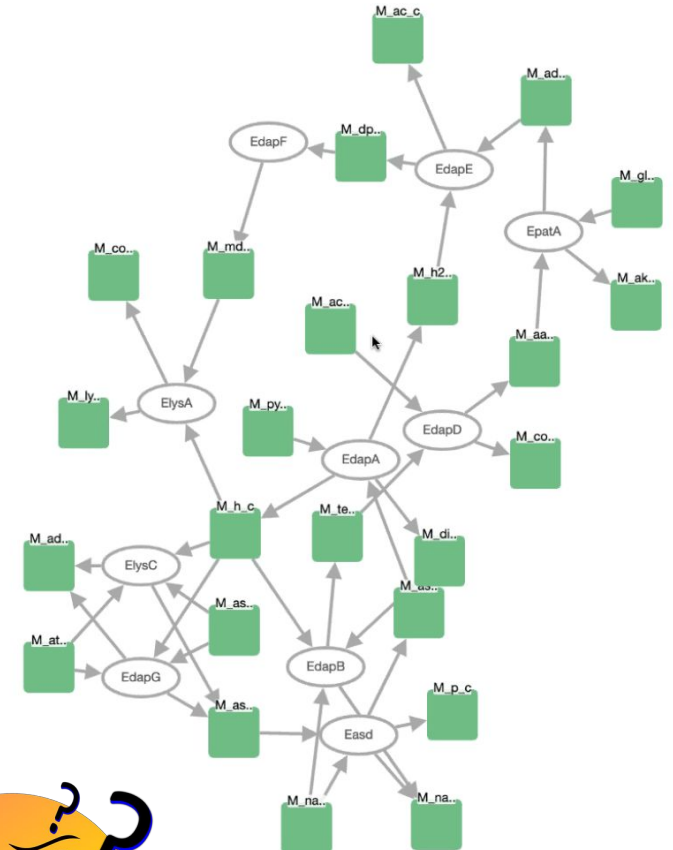
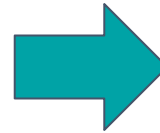
Thomas Duigou



→ Comment représenter les voies métaboliques et les données associées ?



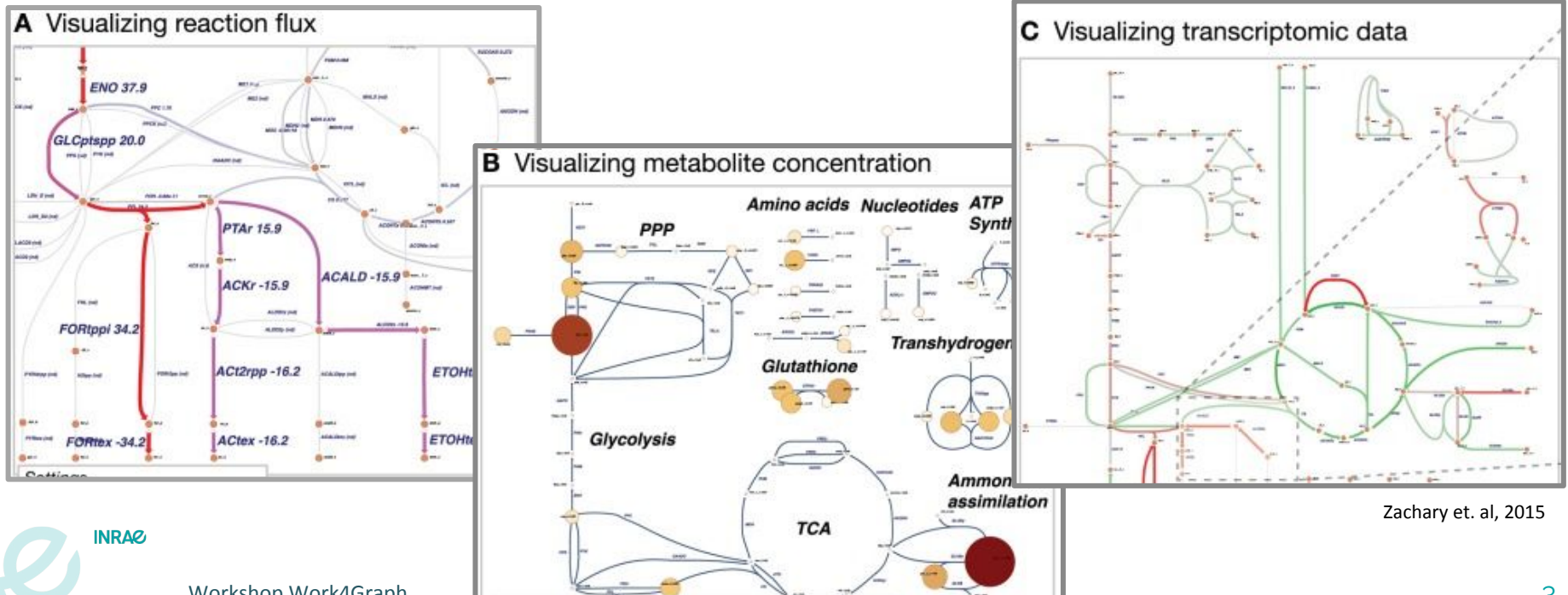
Algorithme "cose"
cytoscape.js



Crédit : Pixabay

→ Publié en 2015 : Zachary A. King, [...], Bernhard O. Palsson, *PLoS Comp Bio*

“Escher: A Web Application for Building, Sharing, and Embedding Data-Rich Visualizations of Biological Pathways”

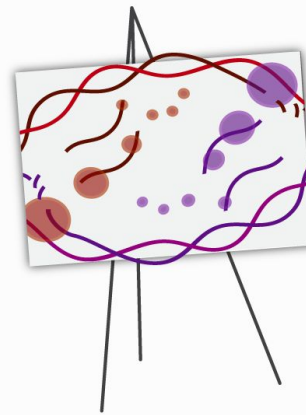


Zachary et. al, 2015

Escher

→ Site web

<https://escher.github.io>



ESCHER

Build, share, and embed visualizations of metabolic pathways

Filter by organism

All

Map

Core metabolism (e_coli_core)

Model (Optional)

e_coli_core

Tool

Builder

Options

- Scroll to zoom (instead of scroll to pan)
- Never ask before reloading

Load map

Demos

Technical demos for developers

Structures

Embed chemical structures

Tooltips

Customize tooltips

Node	Value
S	2
U	1
C	1
O	1
A	1

Escher

→ Documentation : <https://escher.readthedocs.io>

Escher
latest

Search docs

1. Getting started with Escher visualizations
2. Tips and Tricks
3. Escher, COBRA, and COBRAPy
4. Escher Python tutorial
5. Validate Escher maps
6. Developing with Escher
7. Developer Tutorial: Custom tooltips
8. EscherConverter
9. JavaScript API
10. Python API
11. License

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Thank you! ❤️

Docs » Welcome to the documentation for Escher

[Edit on GitHub](#)

Welcome to the documentation for Escher

Escher is a web-based tool for building, viewing, and sharing visualizations of metabolic pathways. These 'pathway maps' are a great way to contextualize metabolic datasets. The easiest way to use Escher is to browse and build maps on the [Escher website](#). New users may be interested in the [Getting started with Escher visualizations](#) guide. Escher also has a [Python package](#) and, for developers, a [NPM package](#).

Escher in 3 minutes

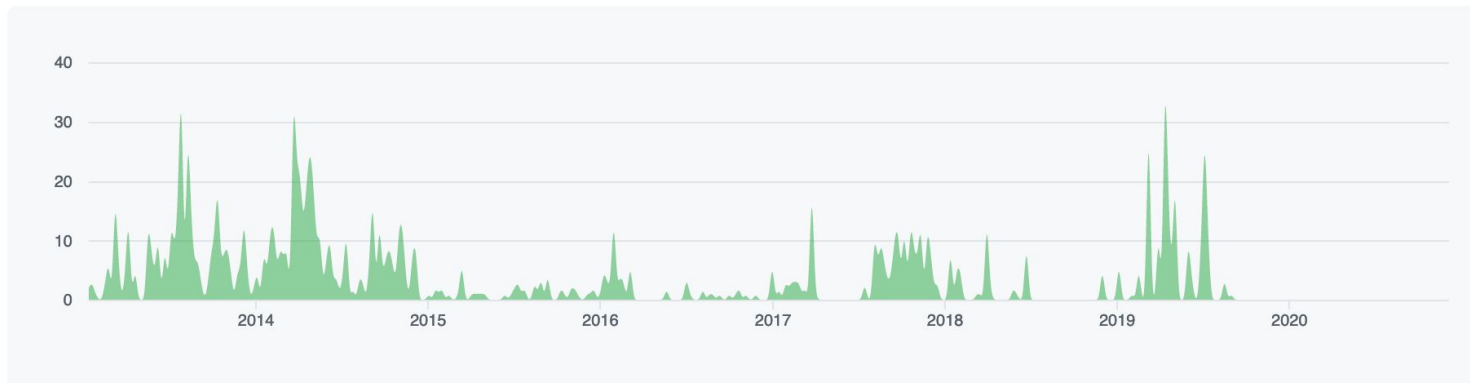


Escher

→ Code source (licence MIT) : <https://github.com/zakandrewking/escher>

The screenshot shows the GitHub repository page for 'zakandrewking / escher'. At the top, there are buttons for 'Watch' (13), 'Star' (138), and 'Fork' (61). Below these are navigation tabs for 'Code', 'Issues' (35), 'Pull requests' (13), 'Actions', 'Projects', and 'Wiki'. A dropdown menu shows 'master' as the selected branch. There are buttons for 'Go to file', 'Add file', and a green 'Code' button. A commit message is visible: 'zakandrewking be sure to redraw after ...' on Sep 5, 2019, with 1,568 views. To the right, the 'About' section describes the project as a tool to 'Build, share, and embed visualizations of metabolic pathways.'

Contributions to master, excluding merge commits



Visualisation web

→ <https://escher.github.io>

The screenshot shows the web interface for visualizing metabolic maps. It includes a search bar for organisms, a section for selecting a map and model, and a 'Load map' button. Numbered callouts (1-4) highlight specific elements: 1. The organism search bar containing 'Escherichia coli'. 2. The 'Map' dropdown menu showing 'Fatty acid biosynthesis (saturate)'. 3. The 'Model (Optional)' dropdown menu showing 'iJO1366'. 4. The 'Load map' button. Callout 1 has an arrow pointing to a dropdown menu with options: 'All', '✓Escherichia coli', 'Homo sapiens', and 'Saccharomyces cerevisiae'. Callout 2 has an arrow pointing to a dropdown menu with options: 'None', 'Core metabolism (e_coli_core)', 'Central metabolism (iJO1366)', 'Fatty acid beta-oxidation (iJO1366)', '✓Fatty acid biosynthesis (saturated) (iJO1366)', 'Nucleotide and histidine biosynthesis (iJO1366)', and 'Nucleotide metabolism (iJO1366)'. Callout 3 has an arrow pointing to a dropdown menu with options: 'None', 'e_coli_core', and '✓iJO1366'. Callout 4 has an arrow pointing to the 'Load map' button.

Filter by organism

Escherichia coli

Map **Model (Optional)** **Tool**

Fatty acid biosynthesis (saturate) iJO1366 Builder

Options

Scroll to zoom (instead of scroll to pan)
 Never ask before reloading

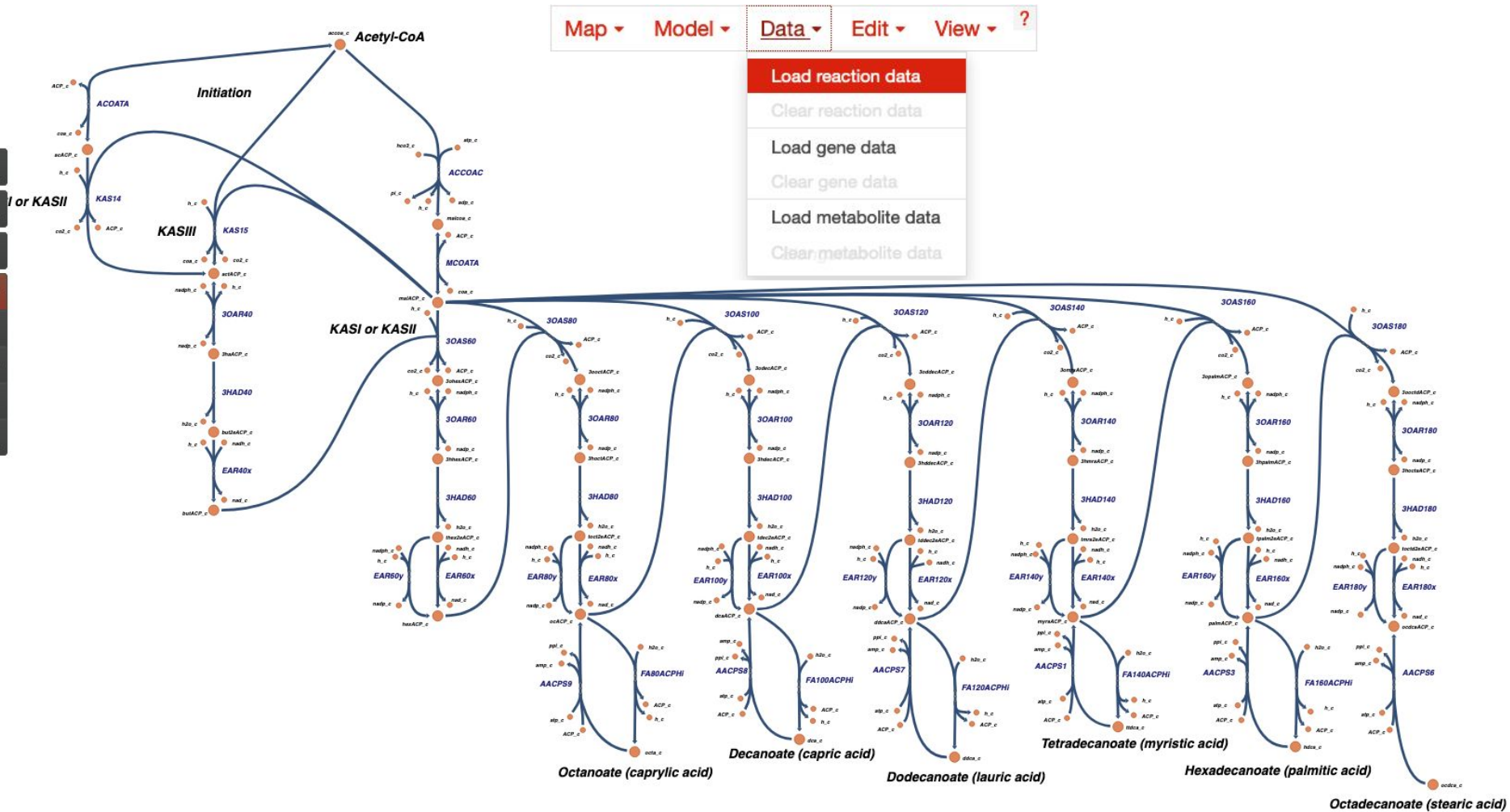
Load map

None
Core metabolism (e_coli_core)
Central metabolism (iJO1366)
Fatty acid beta-oxidation (iJO1366)
✓Fatty acid biosynthesis (saturated) (iJO1366)
Nucleotide and histidine biosynthesis (iJO1366)
Nucleotide metabolism (iJO1366)

None
e_coli_core
✓iJO1366

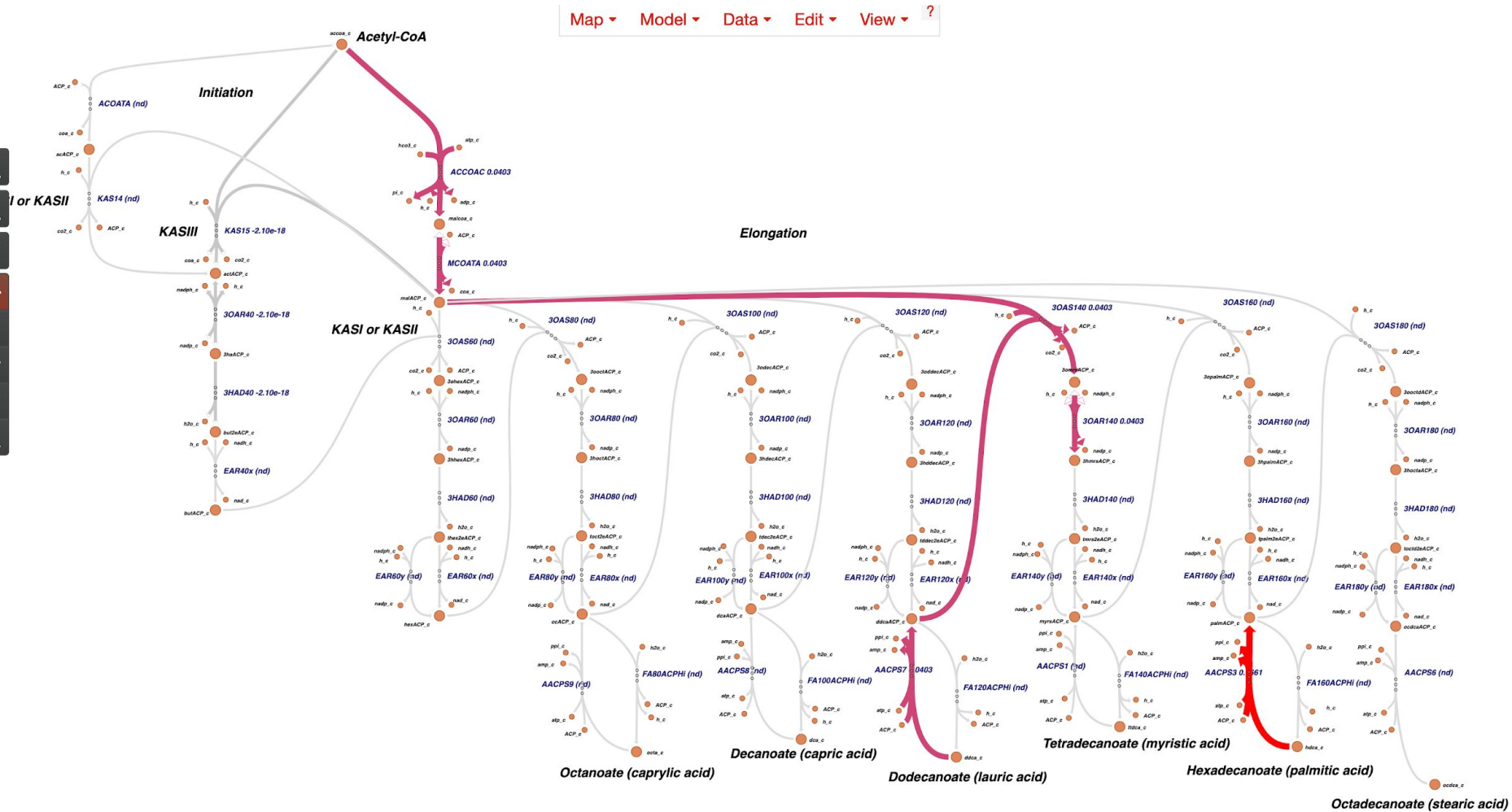
Visualisation web

→ <https://escher.github.io>



Visualisation web

→ Données liées aux réactions

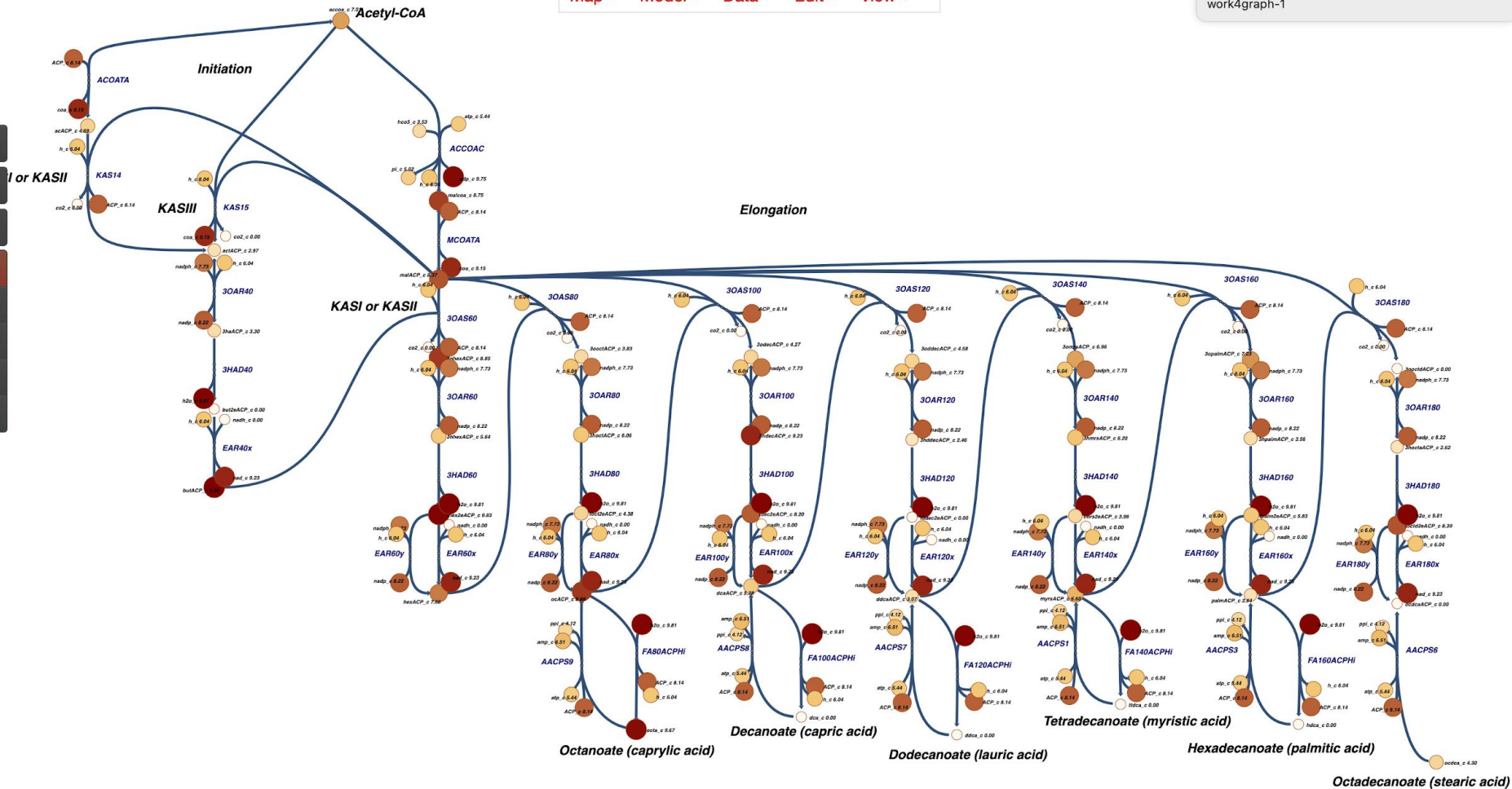


Visualisation web

→ Données liées aux métabolites

Map ▾ Model ▾ Data ▾ Edit ▾ View ▾ ?

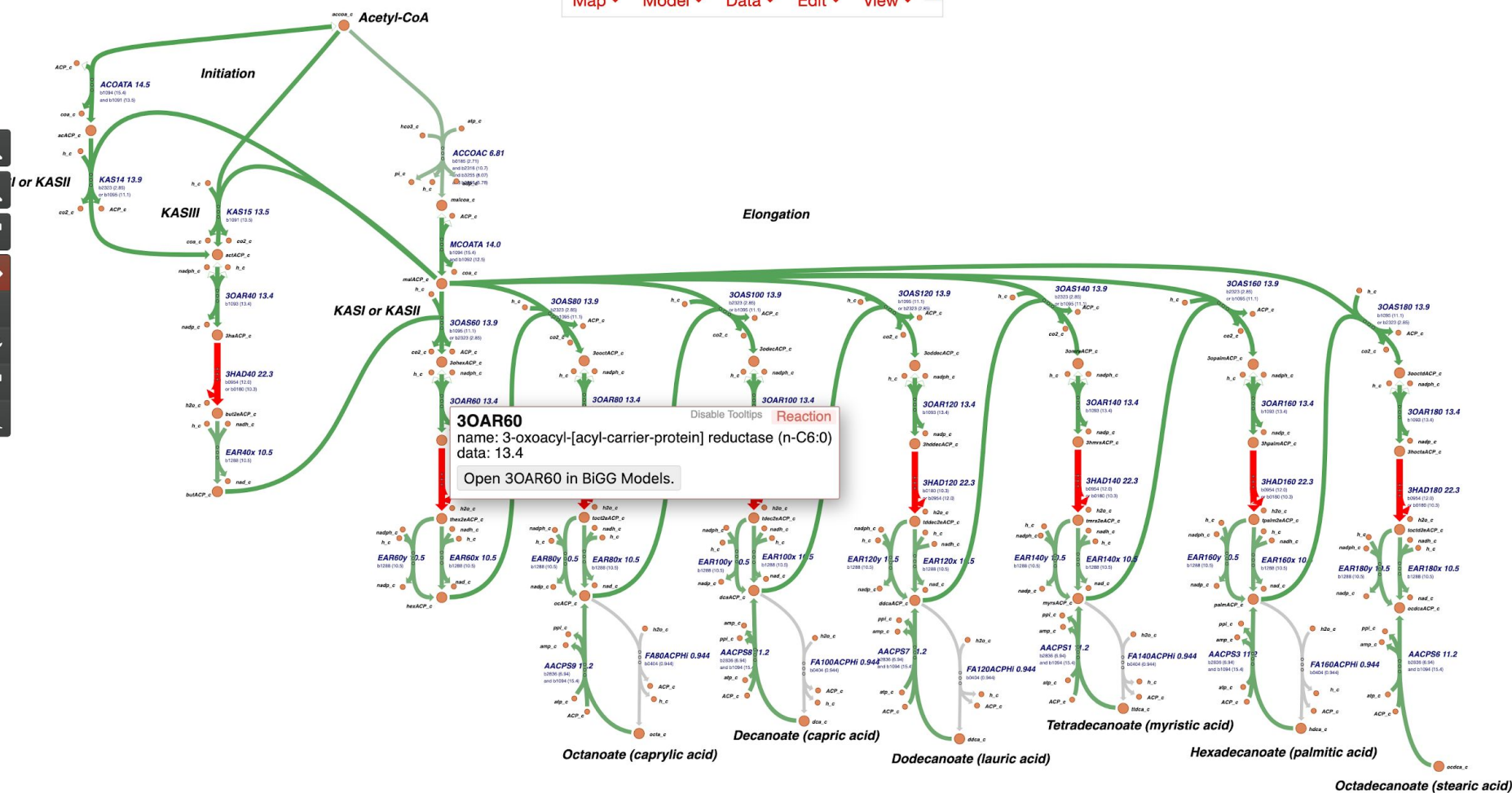
<https://www.gotomeet.me/CatiSysmics/work4graph-1>



Visualisation web

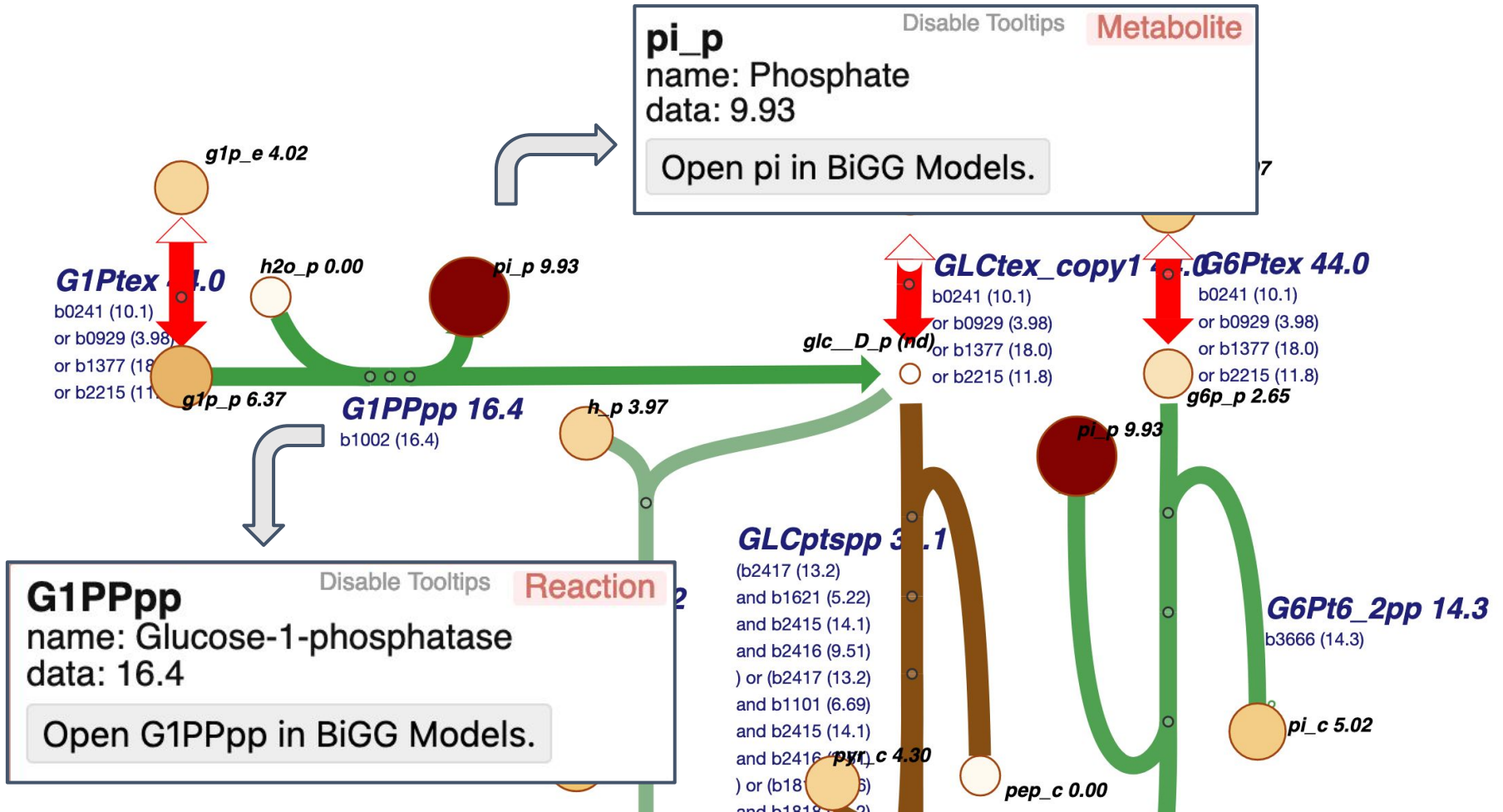
→ Données liées aux gènes

Map ▾ Model ▾ Data ▾ Edit ▾ View ▾ ?



Visualisation web

→ Info-bulles



Visualisation web

→ Personnalisation de la vue

View and build options

Identifiers: ID's Descriptive names

- Scroll to zoom (instead of scroll to pan)
- Hide secondary metabolites
- Show gene reaction rules
- Hide reaction, gene, and metabolite labels
- Allow duplicate reactions
- Highlight reactions not in model
- Use 3D transform for responsive panning and zooming


Show tooltips over: Labels Objects

Tip: To increase map performance, turn off text boxes (i.e. labels and gene reaction rules).

Reactions

Preset Scale Selections ▾

To add a color stop to the scale, click the gradient



Value: 0.01 20 max (43.99)

Color: #9696ff #209123 #ff0000

Size: 16 20 25

Styles for reactions with no data

Color: #dcdcdc Size: 8

Reaction or Gene data

Options: Absolute value Size Color
 Text (Show data in label)


Comparison: Fold Change Log2 (Fold Change) Difference

Method for evaluating AND: Mean Min

Metabolites

Preset Scale Selections ▾

To add a color stop to the scale, click the gradient



Value: min (0) median (6.04) max (9.99)

Color: #ffffaf #f1c470 #800000

Size: 20 30 40

Styles for reactions with no data

Color: #ffffff Size: 10

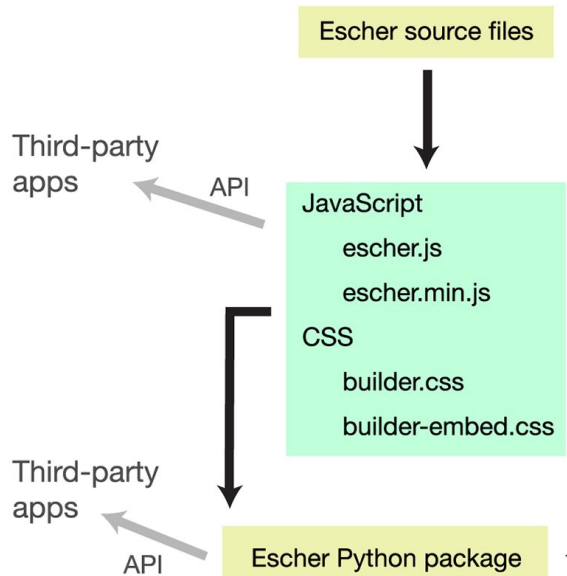
Metabolite data

Options: Absolute value Size Color
 Text (Show data in label)

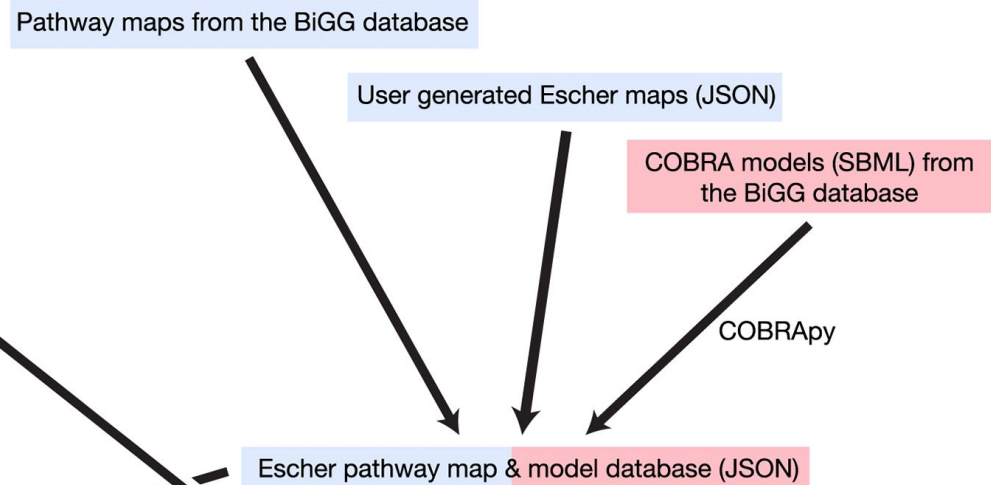
Comparison: Fold Change Log2 (Fold Change) Difference

Organisation de l'outil

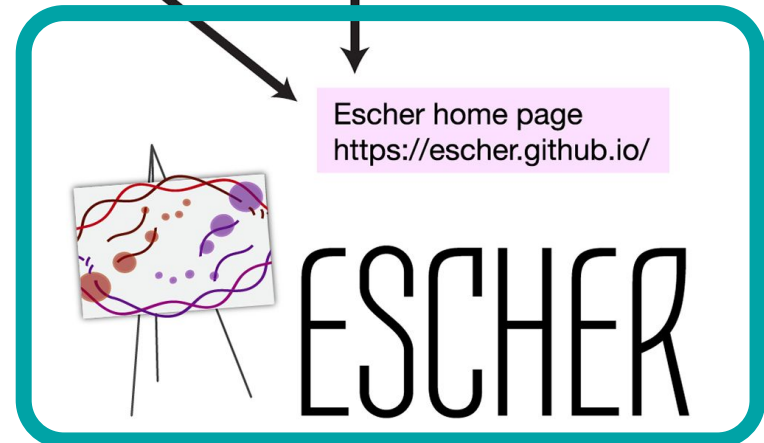
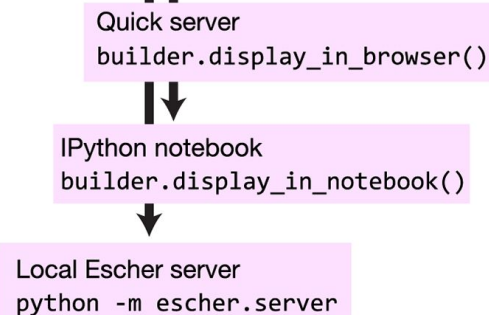
A Escher software



B Pathway maps and COBRA models

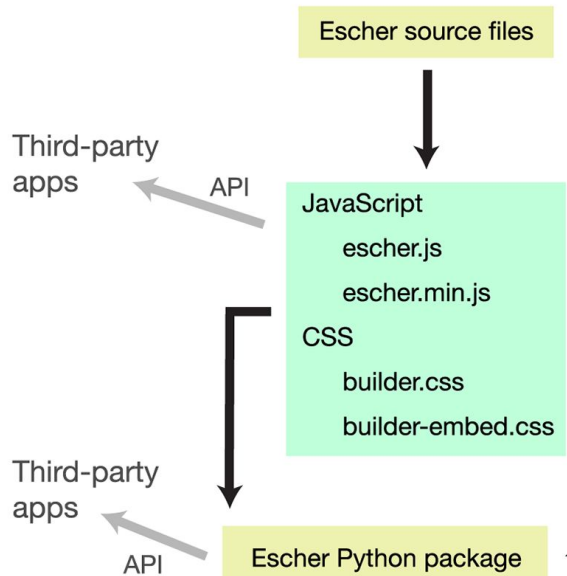


C The Escher web application

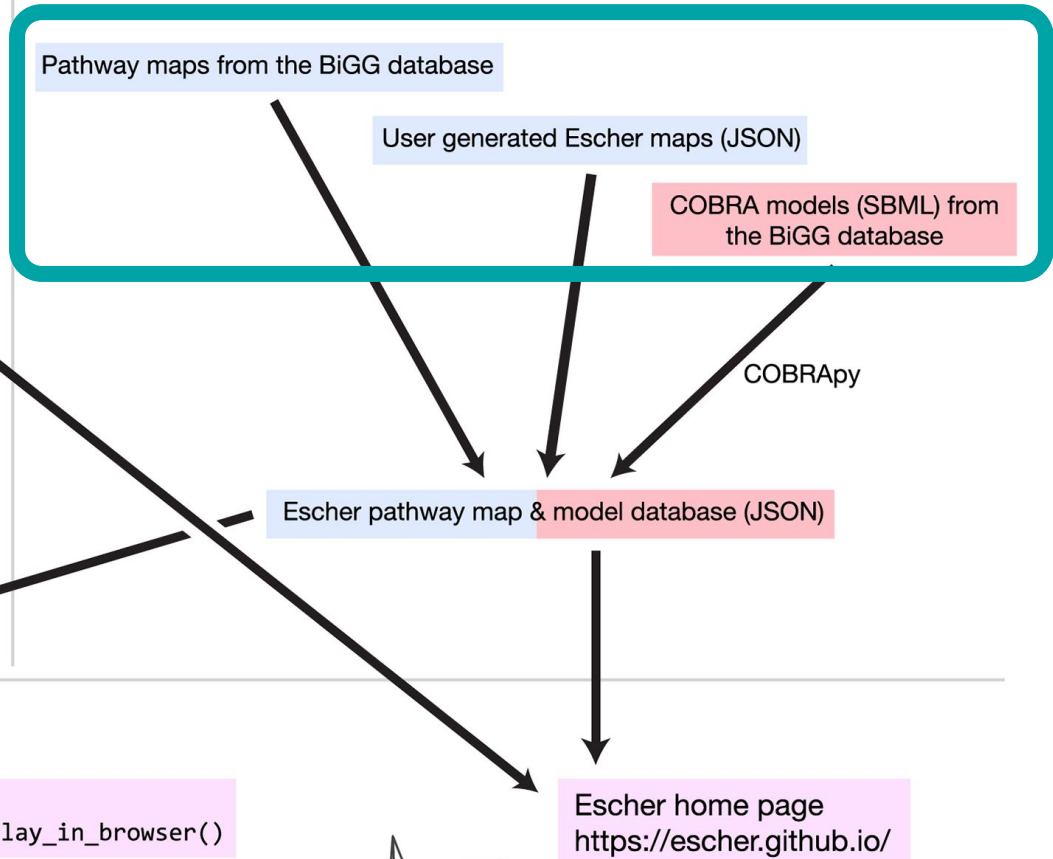


Organisation

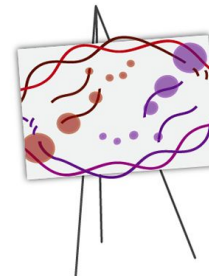
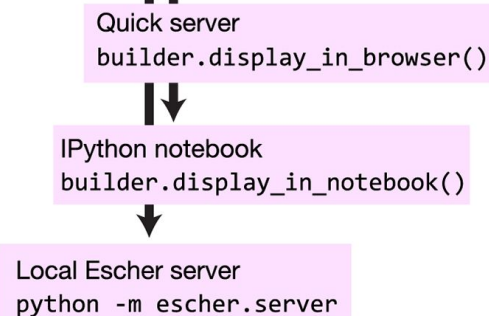
A Escher software



B Pathway maps and COBRA models



C The Escher web application



ESCHER

BiGG : collections de modèles SBML

→ <http://bigg.ucsd.edu/>

BiGG Models

Search the database by model, reaction, metabolite, or gene ?

Search

Exclude multi-strain models from search

Latest update Version 1.6: Adds 23 new models & more!

View Models

View Metabolites

View Reactions

→ Collection d'identifiants "universels" de composés et réactions

Universal metabolite: **glu__L**

Descriptive name:

L-Glutamate

Formulae in BiGG models:

C5H8NO4

Charges in BiGG models:

0,-1

glu__L in BiGG models:

Organism	Model
Escherichia coli str. K-12 substr. MG1655	iJO1366
Escherichia coli str. K-12 substr. MG1655	iAF1260
Saccharomyces cerevisiae S288C	iMM904
Staphylococcus aureus subsp. aureus N315	iSB619

External database links

InChI Key: [WHUUTDBJXJRKMK-VKHYMYHEASA-M](#)

Reactome Compound: [113552](#), [210382](#), [29404](#), [428614](#)

SEED Compound: [cpd00023](#), [cpd19002](#), [cpd27177](#)

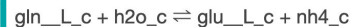
CHEBI: [CHEBI:13107](#), [CHEBI:14321](#),

Universal reaction: **GLUN**

Descriptive name:

Glutaminase

Reaction:



Metabolites:

Stoichiometry	BiGG ID	Name
-1.0	gln_L_c	L-Glutamine
1.0	glu_L_c	L-Glutamate
-1.0	h2o_c	H2O H2O
1.0	nh4_c	Ammonium

GLUN in BiGG models:

Organism	Model
Escherichia coli str. K-12 substr. MG1655	e_coli_core
Escherichia coli str. K-12 substr. MG1655	iAF1260
Escherichia coli str. K-12 substr. MG1655	iAF1260b

External database links

RHEA: [15889](#), [15890](#), [15891](#), [15892](#)

KEGG Reaction: [R00256](#)

BioCyc: [META:GLUTAMIN-RXN](#)

Reactome Reaction: [R-BTA-70609](#), [R-CEL-70609](#), [R-CFA-70609](#), [R-DDI-70609](#), [R-DME-70609](#), [R-DRE-70609](#), [R-GGA-70609](#), [R-HSA-70609](#), [R-MMU-70609](#), [R-RNO-70609](#), [R-SSC-70609](#), [R-TGU-70609](#), [R-XTR-70609](#)

EC Number: [1.4.1.13](#), [1.4.7.1](#), [3.5.1.2](#), [3.5.1.38](#), [4.3.3.6](#), [6.3.4.2](#), [6.3.5.2](#), [6.3.5.4](#), [6.3.5.5](#)

SEED Reaction: [rxn00189](#)

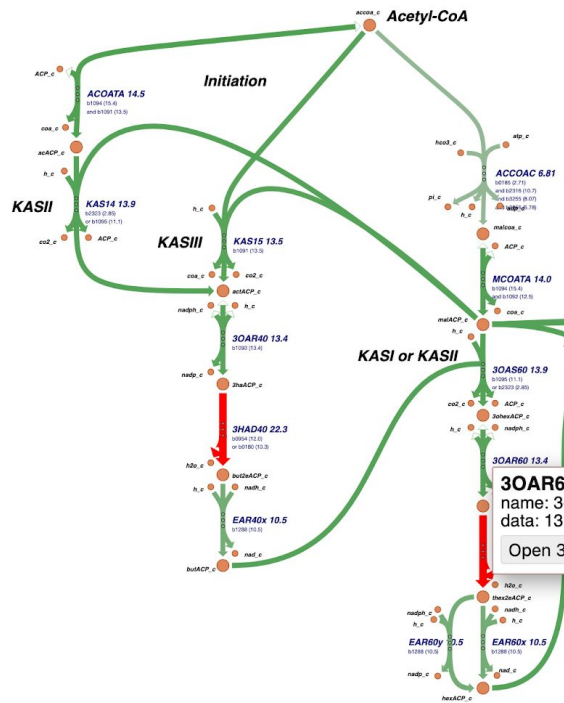
MetaNetX (MNX) Equation: [MNXR100030](#)

Provided by MetaNetX (CC BY 4.0)

Old identifiers

[GLUN](#), [HMR_9802](#)

Cartes de référence



Vue dans Escher

=

```

1 {
2   "reactions": {
3     "2075839": {
4       "name": "Malate dehydrogenase",
5       "bigg_id": "MDH",
6       "reversibility": true,
7       "label_x": 3019.1480390625,
8       "label_y": 3883.49973125,
9       "gene_reaction_rule": "b3236",
10      "genes": [
11        {
12          "bigg_id": "b3236",
13          "name": "mdh"
14        }
15      ],
16      "metabolites": [
17        {
18          "coefficient": -1,
19          "bigg_id": "mal__L_c"
20        },
21        {
22          "coefficient": 1,
23          "bigg_id": "h_c"
24        },
25        {
26          "coefficient": -1,
27          "bigg_id": "nad_c"
28        },
29        {
30          "coefficient": 1,
31          "bigg_id": "oaa_c"
32        },
33        {
34          "coefficient": 1,
35          "bigg_id": "nadh_c"
36        }
37      ]
38    },
39    ...
40  }

```

Carte de référence

+

```

1 {
2   "PMEACPE": 0.00000104,
3   "GLYCLTtex": -0.00034642,
4   "D-LACT2pp": 6.33e-26,
5   "UAMAGS": 0.014389,
6   "RNTR3c2": 0.01399,
7   "DDPA": 0.19735,
8   "Htex": -55.4374,
9   "ADNtex": -9.35e-26,
10  "DHPS2": 0.00034642,
11  "UPP3MT": 0.00011547,
12  "BMOCOS": 0.0000632,
13  "ACACT4r": 0.18428,
14  "EX_lac__D_e": -6.33e-26,
15  "P5CR": 0.11447,
16  "TMPPP": 0.00011547,
17  "ATPM": 3.15,
18  "EX_glyclt_e": 0.00034642,
19  "GLUTRR": 0.0018476,
20  "GLUTRS": 0.0018476,
21  "MN2tpp": 0.00035781,
22  "G1PACT": 0.048928,
23  ...

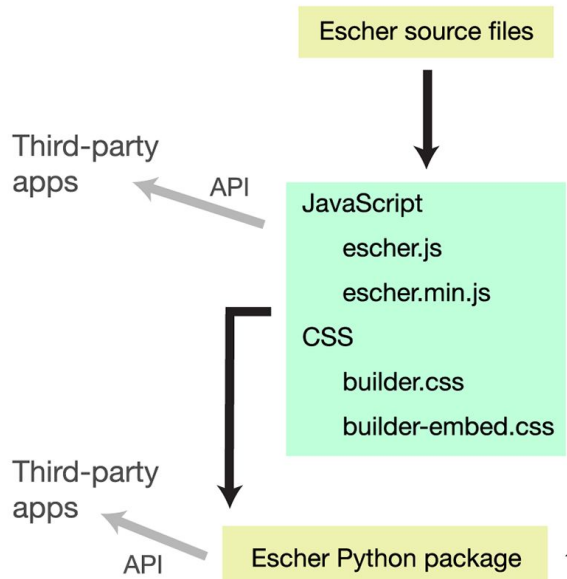
```

Données qualitatives
ou quantitatives

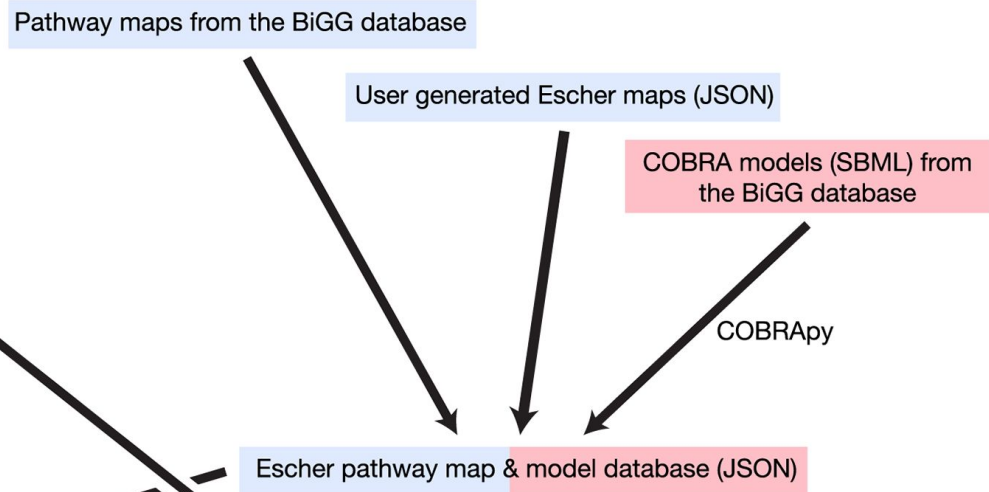
➔ Interface pour construire les cartes de référence manuellement

Organisation

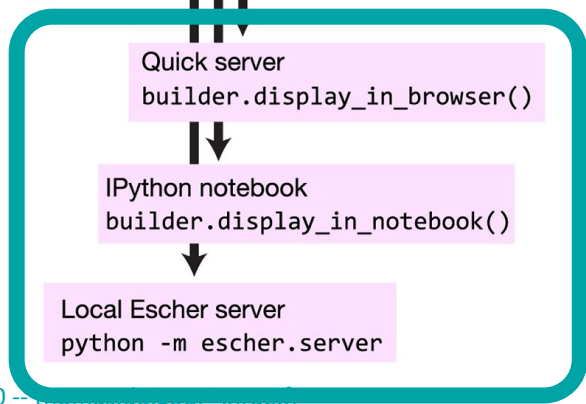
A Escher software



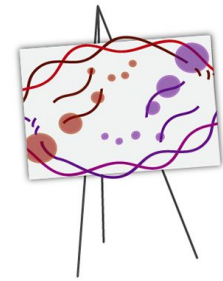
B Pathway maps and COBRA models



C The Escher web application



Escher home page
<https://escher.github.io/>



ESCHER

Escher avec Python & Jupyter

→ Installation

```
conda create -n escher python=3.8  
conda activate escher  
pip install escher
```

→ Exécution

```
conda activate escher  
jupyter notebook escher_tutorial_20201208.ipynb
```

→ Tutoriel (live)

- Code source : <https://sysmics.cati.inrae.fr/work4graph>

- Propose une représentation proche de ce que l'on voit habituellement dans les bases de données / les publications
 - Outil "dynamique", facile à utiliser
 - Open Source et bien documenté
 - Fonctionnalité pour créer ses propres cartes (manuellement)
-
- Cartes de référence en nombre limité
 - Pas d'outil pour générer des cartes automatiquement
 - Représentation des phénomènes de régulation ?
 - Maintenance de l'outil ?

INRAE

> **Merci !**

