

# ATLAS of Biochemistry

USER GUIDE

<http://lcsb-databases.epfl.ch/atlas/>

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## USE IT !

- Fill a gap
- Find a pathway
- Get information

# GET STARTED

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- Send an e-mail to [jasmin.hafner@epfl.ch](mailto:jasmin.hafner@epfl.ch) with
  - Your name
  - Your institution

→ *Please note that only requests from group leaders will be considered!*
- We will send you a license agreement to be signed, and provide you with username & password
- Go to <http://lcsb-databases.epfl.ch/atlas/> and login:



Please Login

Username :

Password :

LOGIN

# NAVIGATE

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## 1. BNICE.ch curated KEGG reactions

A table of **6'651** KEGG reactions, curated by BNICE.ch and computationally annotated with values for the **Gibbs free energy of reactions**, a 3<sup>rd</sup> level **EC number** and a reconstruction mode

## 2. BNICE.ch ATLAS reactions

A table of **137'877** known and novel enzymatic reactions, annotated with values for the **Gibbs free energy of reactions**, a 3<sup>rd</sup> level **EC number** and, for novel reactions, the structurally **most similar KEGG reaction** including similarity score (BridgIt result)

## 3. Pathways

A tool to perform a **pathway search** from a source compound to a target compound

## 4. Maps

A tool to explore the **metabolic neighborhood** of a source compound

# 1. CURATED KEGG REACTIONS

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Choose visible columns

Export reactions as a CSV file

Show selected sets of reactions

Sort alphabetically

Search for a string

HOMEPAGE ATLAS **BNICE.ch CURATED KEGG REACTIONS** BNICE.ch ATLAS REACTIONS PATHWAYS MAP LOGIN

BNICE.ch Curated KEGG Reactions

Column visibility Export all Export selected rows Show exact reconstructions Show one-step covered reactions Show multi-step reactions Search:

KEGG	REACTION	NAME	ENZYME	REACTION RULE	ENERGY	ERR	RECONSTRUCTION
R00192	C00001+C00021 ↔ C00189+C00212	S-Adenosyl-L-homocysteine hydrolase	3.3.1.1	3.3.1.-	-5.67	true	exact reconstruction
R00193	C00001+C00021 ↔ C00014+C00431	S-Adenosyl-L-homocysteine aminohydrolase	3.5.4.28	3.5.99.-	-5.62	true	exact reconstruction
R00194	C00001+C00021 ↔ C00147+C00039	S-Adenosyl-L-homocysteine homocysteine-ribosylhydrolase	3.2.2.8	3.2.2.-	-6.73	true	exact reconstruction
R00196	C00001+C00095 ↔ 2 C00014+C00022	2,3-diaminopropionate ammonia-lyase (adding water, pyruvate-forming)	4.3.1.15	4.3.1.-	-21.62	true	exact reconstruction
R00199	C00001+C00002+C00022 ↔ C00008+C00025+C00016	ATP:pyruvate:water phosphotransferase	2.7.9.2		0	false	1-step biotransformation
R00200	C00002+C00022 ↔ C00008+C00016	ATP:pyruvate 2-O-phosphotransferase	2.7.1.40	2.7.1.-	-4.61	true	exact reconstruction

KEGG ID Reaction equation

Name of the enzyme (if known)

EC number according to KEGG

3<sup>rd</sup> – level EC number according to ATLAS

Gibbs free energy of reaction in kJ/mol + error

Level of reconstruction in ATLAS

## 2. ATLAS REACTIONS

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Choose visible columns

Export reactions as a CSV file

Sort alphabetically

Search for a string

BNICE.ch ATLAS Reactions

Column visibility Export Export selected row Search

ATLAS	KEGG	REACTION	REACTION RULE	ENERGY	ERR	MOST SIM. KEGG	BRIDGIT
h000401	R03942	C00003+C02431 <=> C02991+C00004+C00080	1.1.1.- 1.2.1.-	-2	0.36		
h000402	R03963	C00004+C02648+C00080 <=> C00003+C02497	1.1.1.- 1.2.1.-	-5.22	0.09		
h000403		C00033+C00004+C00080 <=> C03264+C00003	1.1.1.- 1.2.1.-	-6.22	0.11	R03069 / 1.1.1.06	0.97
h000404		C02780+C00004+C00080 <=> C03342+C00003	1.1.1.- 1.2.1.-	-3.76	0.18	R08879 / 1.1.1.274 1.1.340	1
h000406		C00004+C04875+C00080 <=> C03342+C00003	1.1.1.- 1.2.1.-	-6.22	0.11	R01899 / 1.1.1.42	0.90
h000406		C04280+C00003 <=> C04873+C00004+C00080	1.1.1.- 1.2.1.-			R10130 / 1.1.1.329	0.95
h000407		C00004+C09893+C00080 <=> C00003+C02484	1.1.1.- 1.2.1.-	-0.75	0.09	R02177 / 1.1.1.207	0.94
h000408	R10189  R10232	C02989+C00003 <=> C00004+C01181+C00080	1.1.1.- 1.2.1.-				
h000408	R10422	C01876+C00004+C00080 <=> C00003+C02945	1.1.1.- 1.2.1.-	-2.3	0.09		

ATLAS ID + KEGG  
ID (if existing)

Reaction equation

3<sup>rd</sup> – level EC number  
according to ATLAS

Gibbs free  
energy of  
reaction in  
kJ/mol + error

Most similar KEGG  
reaction incl. EC number +  
BridgIT similarity score  
(1 = same, 0 = no similarity)

### 3. PATHWAYS - Overview

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#### Atlas Pathways

Search for all the possible routes from any substrate compound to any product.

Maximal number of pathways	200
Maximal pathway length	5
Maximal number of novel intermediates	4
Maximal change in carbon flow	1
Source compound ID	17476
Source compound name/KEGG	Caffeine (C07461)
Target compound ID	13315
Target compound name/KEGG	Theobromine (C07460)

Search for Pathways

Set the maximum number of pathways to show, the maximum pathway length, the maximum number of novel steps, and the maximal change in carbon atoms

Type in the name or the KEGG ID of the source compound and the target compound

KEGG score =  
# KEGG reactions / # reaction steps

Length score =  
1 / # reaction steps

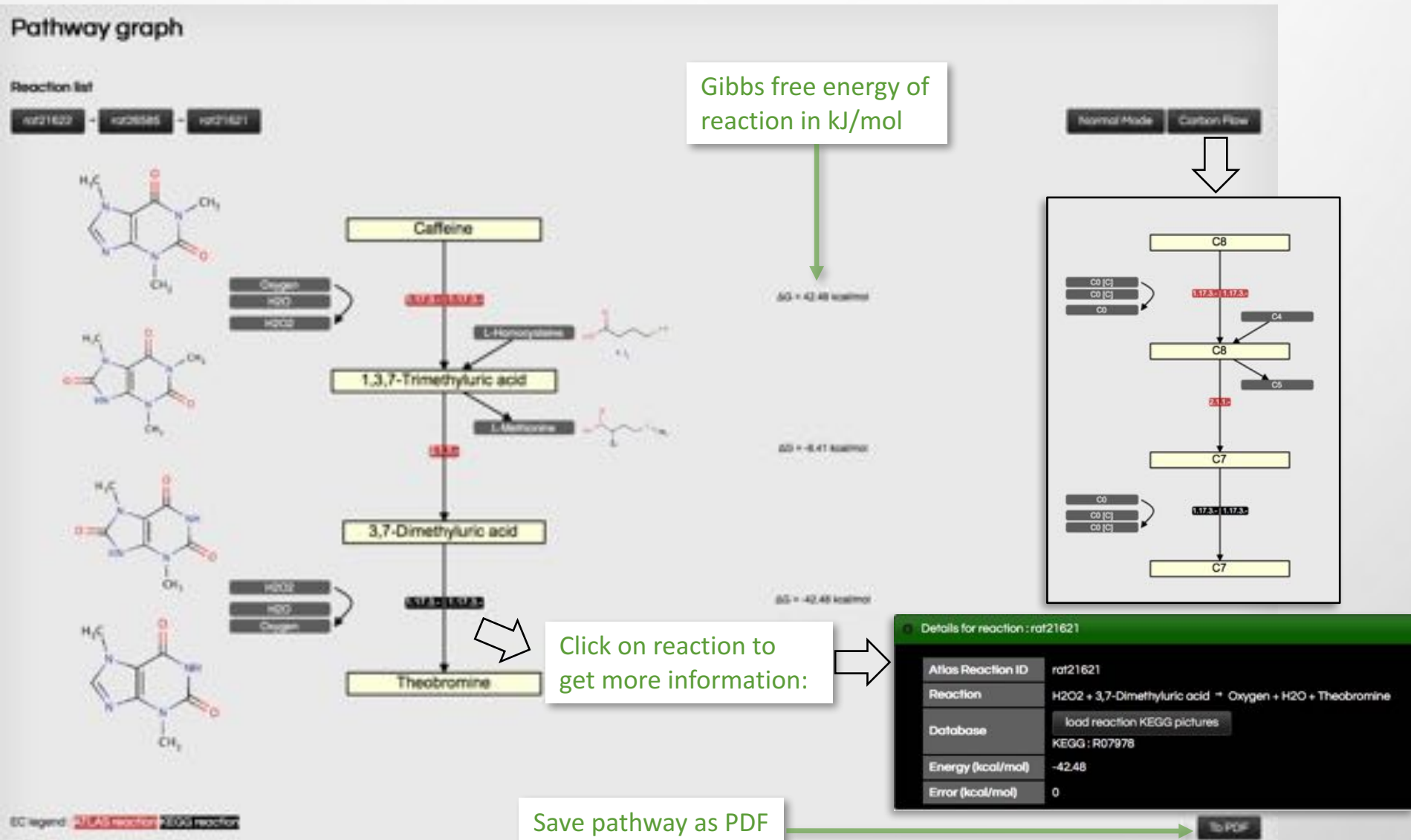
Graph visualization

Column visibility Export CSV Export selected

ID	LENGTH	INTERMEDIATES KEGG	INTERMEDIATE NAMES	REACTIONS	LENGTH SC.	KEGG SC.	GRAPH
1	1	C07461 ↔ C07460	Caffeine ↔ Theobromine	rxn26726	1	0	<a href="#">Graph</a>
2	3	C07461 ↔ C07130 ↔ C16357 ↔ C07460	Caffeine ↔ Theophylline ↔ 3-Methylxanthine ↔ Theobromine	rxn26724, rxn26716, rxn26723	0.33	0	<a href="#">Graph</a>
3	3	C07461 ↔ C13747 ↔ C00155 ↔ C07460	Caffeine ↔ 1,7-Dimethylxanthine ↔ L-Homocysteine ↔ Theobromine	rxn26725, rxn26725, rxn26726	0.33	0	<a href="#">Graph</a>
4	3	C07461 ↔ C13747 ↔ C01217 ↔ C07460	Caffeine ↔ 1,7-Dimethylxanthine ↔ 5,6,7,8-Tetrahydronethopterin ↔ Theobromine	rxn26725, rxn26410, rxn26022	0.33	0	<a href="#">Graph</a>

### 3. PATHWAYS - Graph visualization

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## 4. MAPS - Metabolic environment

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### Atlas Map

The reaction map finds all KEGG compounds connected to a given source compound in one, two or more reaction steps.

Maximal number of reactions in the map: 200

Use neighborhood algorithm for included compounds: ☒ Yes

Add compound by ID

Compound ID: 13315

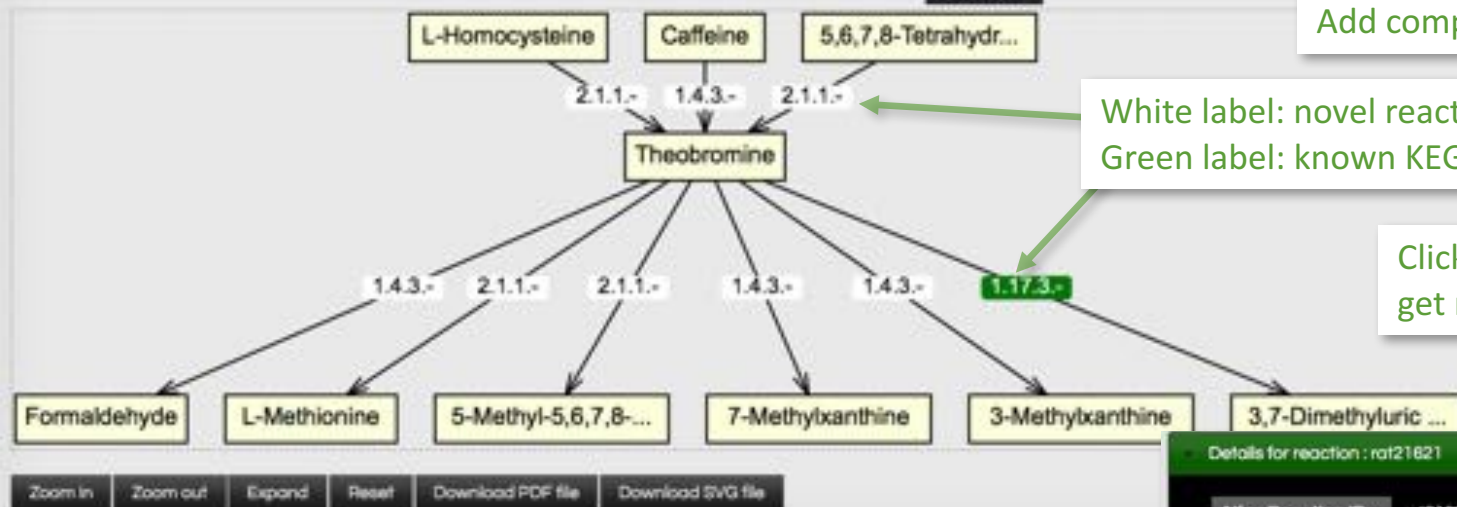
Compound name: Theobromine (C07480)

Load Map

Set a maximum number of pathways to show, as well as a maximum number of reactions steps away from the starting compound

Type in the name of the compound or the KEGG ID

Add compounds to expand the map



White label: novel reaction  
Green label: known KEGG reaction

Click on reaction to get more information:



Details for reaction : rat21621	
Atlas Reaction ID	rat21621
Reaction	H2O2 + 3,7-Dimethyluric acid + Oxygen + H2O + Theobromine
Database	load reaction KEGG pictures KEGG : R07978
Energy (kcal/mol)	-42.48
Error (kcal/mol)	0

Visualization settings

Download the reaction network in PDF or SVG format

# USE IT !

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- **Find a pathway** for a metabolic engineering project.

Use the pathway search to find a new biosynthesis route of known and novel enzymatic reaction steps from a precursor metabolite towards your chemical of interest. For novel reactions, we provide the most similar KEGG reaction which can be used as a starting point for enzyme engineering approaches. The values for the Gibbs Free Energy of reactions help to evaluate the thermodynamic feasibility of a new pathway.

- **Fill a gap** in a metabolic network reconstruction.

Use the pathway search to find possible reaction steps that bridge the gap in your metabolic network. Thanks to the BridgIT annotation you can even find a similar KEGG reactions and trace back a candidate gene sequence by Gene-Protein-Reaction (GPR) association.

- **Get information** about a specific KEGG reaction.

The database of curated KEGG reactions can be used to retrieve information that is missing in other databases, especially regarding EC classification, reaction mechanism for multi-step reactions or Gibbs free energy of reaction.