ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

LABORATORY OF COMPUTATIONAL
SYSTEMS BIOTECHNOLOGY

ATLAS of Biochemistry

USER GUIDE

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

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- Curated KEGG reactions
- ATLAS reactions
- Pathways
- Maps

3

USE IT !

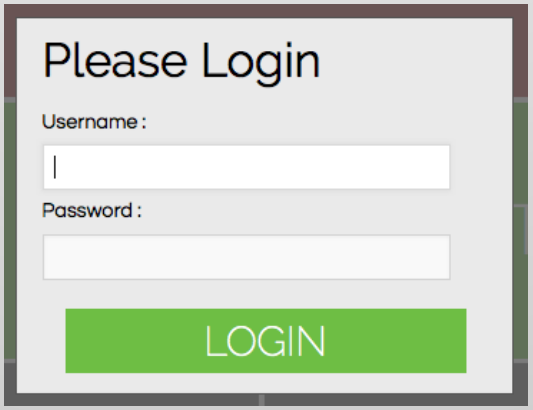
- Fill a gap
- Find a pathway
- Get information

GET STARTED

1

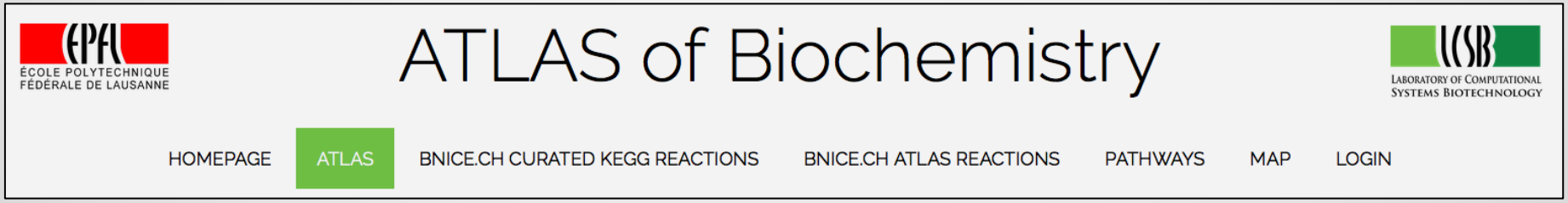
- Send an e-mail to anastasia.sveshnikova@epfl.ch with
  - Your name
  - Your institution

  → ***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:



NAVIGATE

2



1. BNICE.ch curated KEGG reactions

   A table of **8'041** KEGG reactions, curated by BNICE.ch and computationally annotated with a 3rd level **EC number** and a reconstruction mode

2. BNICE.ch ATLAS reactions

   A table of **149'052** known and novel enzymatic reactions, annotated with values for the **Gibbs free energy of reactions**, a 3rd level **EC number** and, for novel reactions, the structurally **most similar known reaction** including a similarity score (BridgIT result)

3. Pathways

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

1. CURATED KEGG REACTIONS

2

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 multistep reactions

Search:

KEGG	REACTION	NAME	ENZYME	REACTION RULE	ENERGY	ERR	RECONSTRUCTION
R00192	C00001+C00021 <=> C00155+C00212	S-Adenosyl-L-homocysteine hydrolase	3.3.1.1	3.3.1.-	-5.67	true	exact reconstruction
R00193	C00001+C00021 <=> C00014+C03431	S-Adenosyl-L-homocysteine aminohydrolase	3.5.4.28	3.5.99.-	-5.82	true	exact reconstruction
R00194	C00001+C00021 <=> C00147+C03539	S-Adenosyl-L-homocysteine homocysteinylribohydrolase	3.2.2.9	3.2.2.-	-0.73	true	exact reconstruction
R00195	C00001+C06393 <=> (2) C00014+C00022	2,3-diaminopropanoate ammonia-lyase (adding water pyruvate-forming)	4.3.1.15	4.3.1.-	-21.62	true	exact reconstruction
R00199	C00001+C00002+C00022 <=> C00009+C00020+C00074	ATP:pyruvate,water phosphotransferase	2.7.9.2		0	false	1-step biotransformation
R00200	C00002+C00022 <=> C00008+C00074	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

3rd – level EC number according to ATLAS

Gibbs free energy of reaction in kcal/mol + error

Level of reconstruc-tion in ATLAS

2. ATLAS REACTIONS

2

Choose visible columns

Export reactions as a CSV file

Sort alphabetically

Search for a string

HOMEPAGE | ATLAS | BNICE.CH CURATED KEGG REACTIONS | BNICE.CH ATLAS REACTIONS | PATHWAYS | MAP | LOGIN

BNICE.ch ATLAS Reactions

Column visibility | Export all | Export selected row

Search:

ATLAS	KEGG	REACTION	REACTION RULE	ENERGY	ERR	MOST SIM. KEGG	BRIDGIT
rat000401	R03942	C00003+C02431 <=> C02991+C00004+C00080	1.1.1.-|1.2.1.-	-2	0.35		
rat000402	R03963	C00004+C02648+C00080 <=> C00003+C02497	1.1.1.-|1.2.1.-	-5.22	0.09		
rat000403		C00233+C00004+C00080 <=> C03264+C00003	1.1.1.-|1.2.1.-	-6.22	0.11	R05068 / 1.1.1.86	0.97
rat000404		C02780+C00004+C00080 <=> C03342+C00003	1.1.1.-|1.2.1.-	-3.76	0.18	R08878 / 1.1.1.274|1.1.1.346	1
rat000405		C00004+C04575+C00080 <=> C03342+C00003	1.1.1.-|1.2.1.-	-6.22	0.11	R01899 / 1.1.1.42	0.98
rat000406		C04280+C00003 <=> C04673+C00004+C00080	1.1.1.-|1.2.1.-			R10130 / 1.1.1.329	0.95
rat000407		C00004+C09893+C00080 <=> C00003+C02484	1.1.1.-|1.2.1.-	-0.75	0.09	R02177 / 1.1.1.207	0.94
rat000408	R10189|R10222	C02489+C00003 <=> C00004+C00161+C00080	1.1.1.-|1.2.1.-				
rat000409	R10422	C01876+C00004+C00080 <=> C00003+C02945	1.1.1.-|1.2.1.-	-2.3	0.09		

ATLAS ID + KEGG ID (if existing)

Reaction equation

3rd – 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 (rat) steps	4
Maximal change in carbon flow	1
Source compound ID	17476
Source compound name/KEGG	Caffeine (C07481)
Target compound ID	13315
Target compound name/KEGG	Theobromine (C07480)

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

Graph visualization

Length score =
1 / # reaction steps

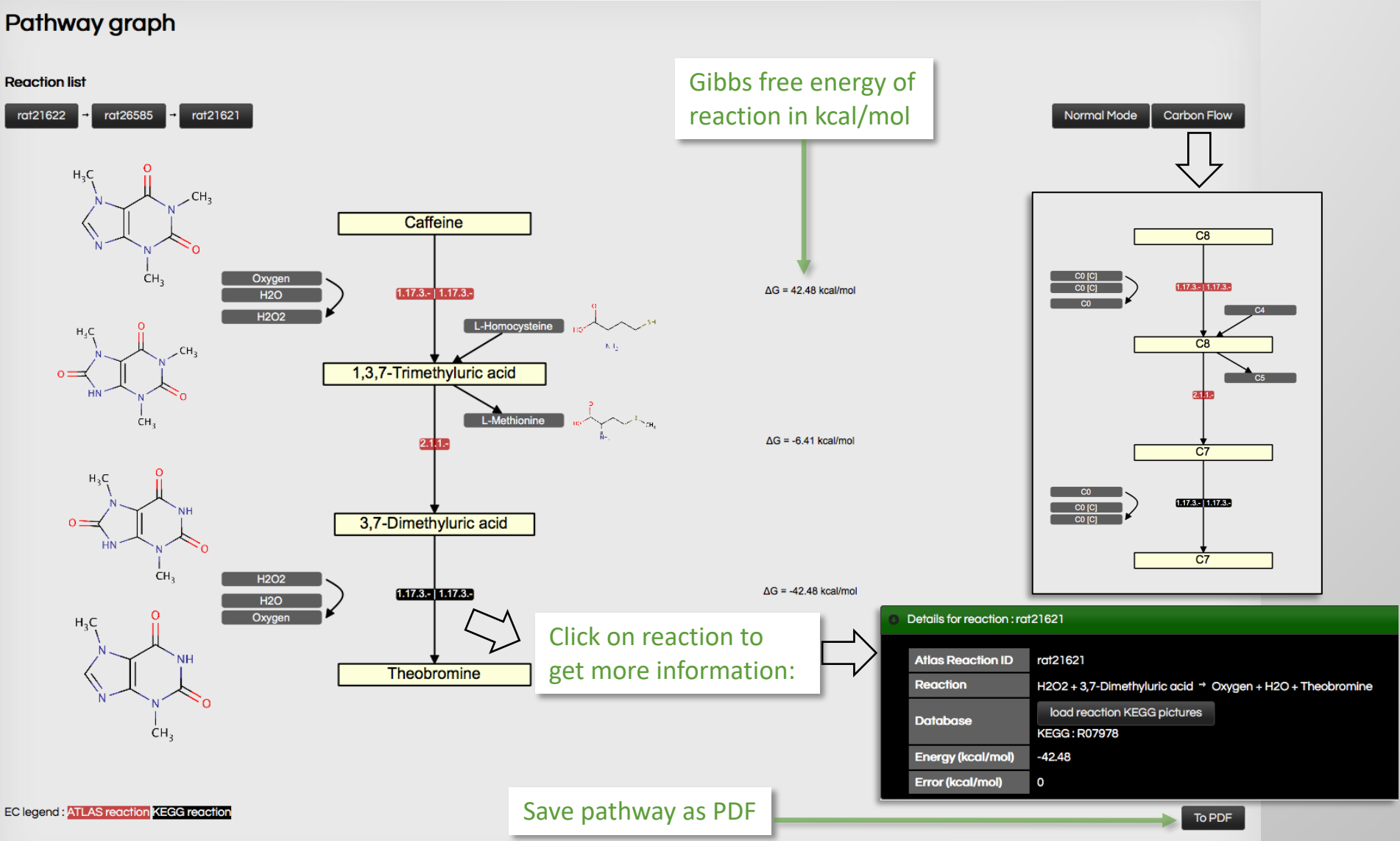
Column visibility | Export CSV | Export selected

Search:

ID	LENGTH	INTERMEDIATES KEGG	INTERMEDIATE NAMES	REACTIONS	LENGTH SC.	KEGG SC.	GRAPH
1	1	C07481 => C07480	Caffeine => Theobromine	rat26726	1	0	Graph
2	3	C07481 => C07130 => C16357 => C07480	Caffeine => Theophylline => 3-Methylxanthine => Theobromine	rat26724, rat26716, rat26723	0.33	0	Graph
3	3	C07481 => C13747 => C00155 => C07480	Caffeine => 1,7-Dimethylxanthine => L-Homocysteine => Theobromine	rat26725, rat26725, rat26726	0.33	0	Graph
4	3	C07481 => C13747 => C01217 => C07480	Caffeine => 1,7-Dimethylxanthine => 5,6,7,8-Tetrahydromethanopterin => Theobromine	rat26725, rat26410, rat26022	0.33	0	Graph

3. PATHWAYS - Graph visualization

2



USE IT !

3

- **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.