ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

LABORATORY OF COMPUTATIONAL
SYSTEMS BIOTECHNOLOGY

ATLAS of Biochemistry

USER GUIDE

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

CONTENT

1

GET STARTED

- Create your user account

2

NAVIGATE

- 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 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:

NAVIGATE

2

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 3rd 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 3rd level **EC number** and, for novel reactions, the structurally **most similar KEGG reaction** including similarity score (BridgIt result)

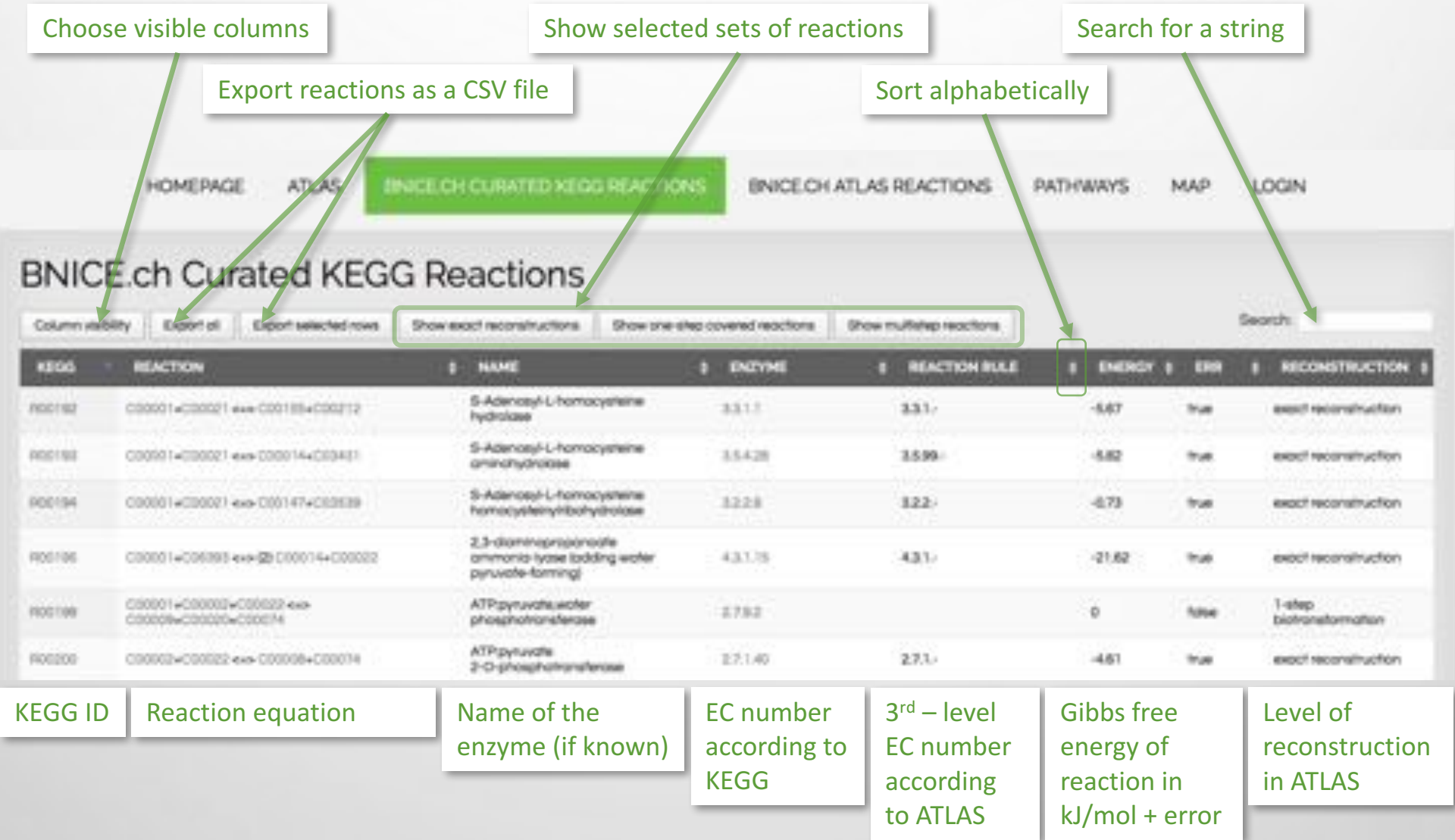
3. Pathways

   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



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 kJ/mol + error

Level of reconstruction in ATLAS

2. ATLAS REACTIONS

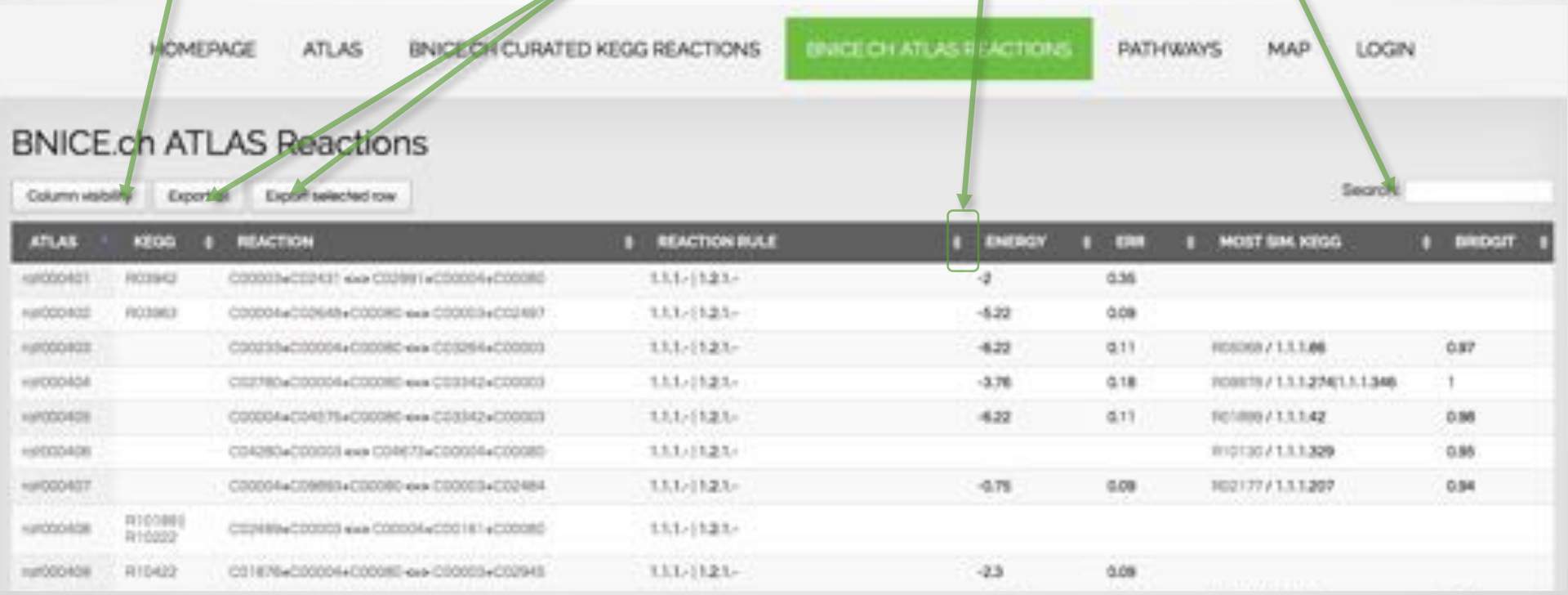
2

Choose visible columns

Export reactions as a CSV file

Sort alphabetically

Search for a string



ATLAS ID + KEGG ID (if existing)

Reaction equation

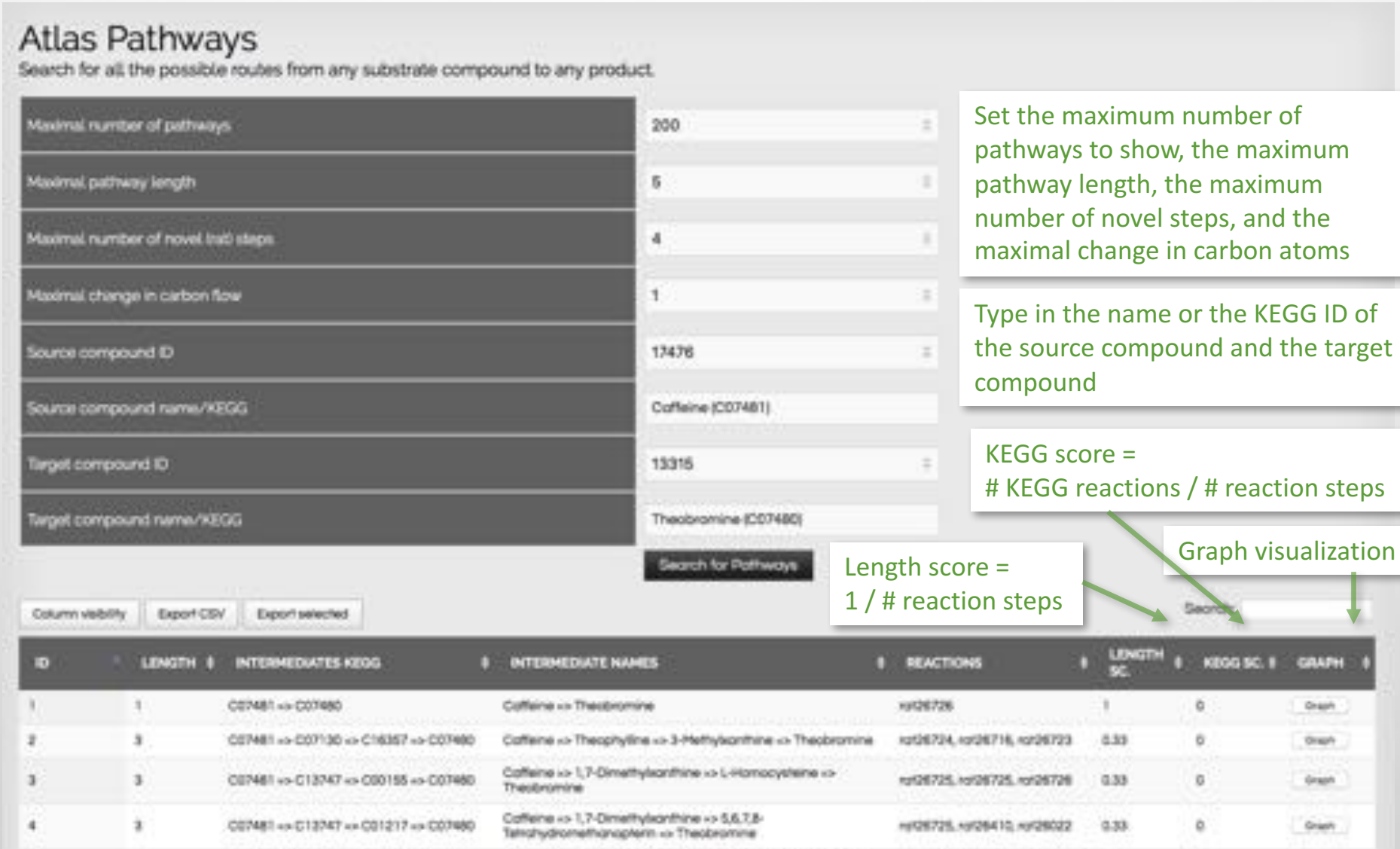
3rd – level EC number according to ATLAS

Gibbs free energy of reaction in kJ/mol + error

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

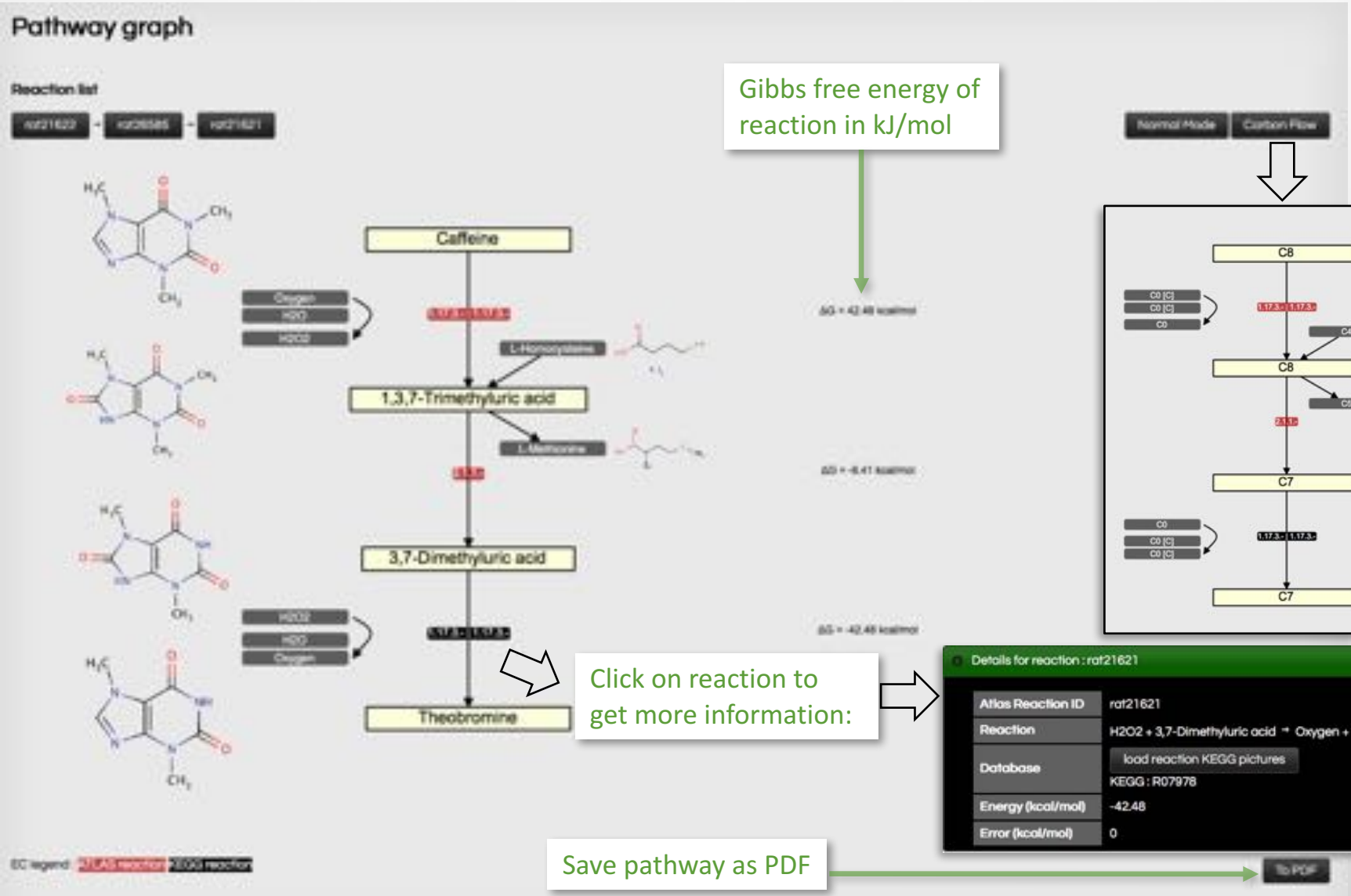
3. PATHWAYS - Overview

2



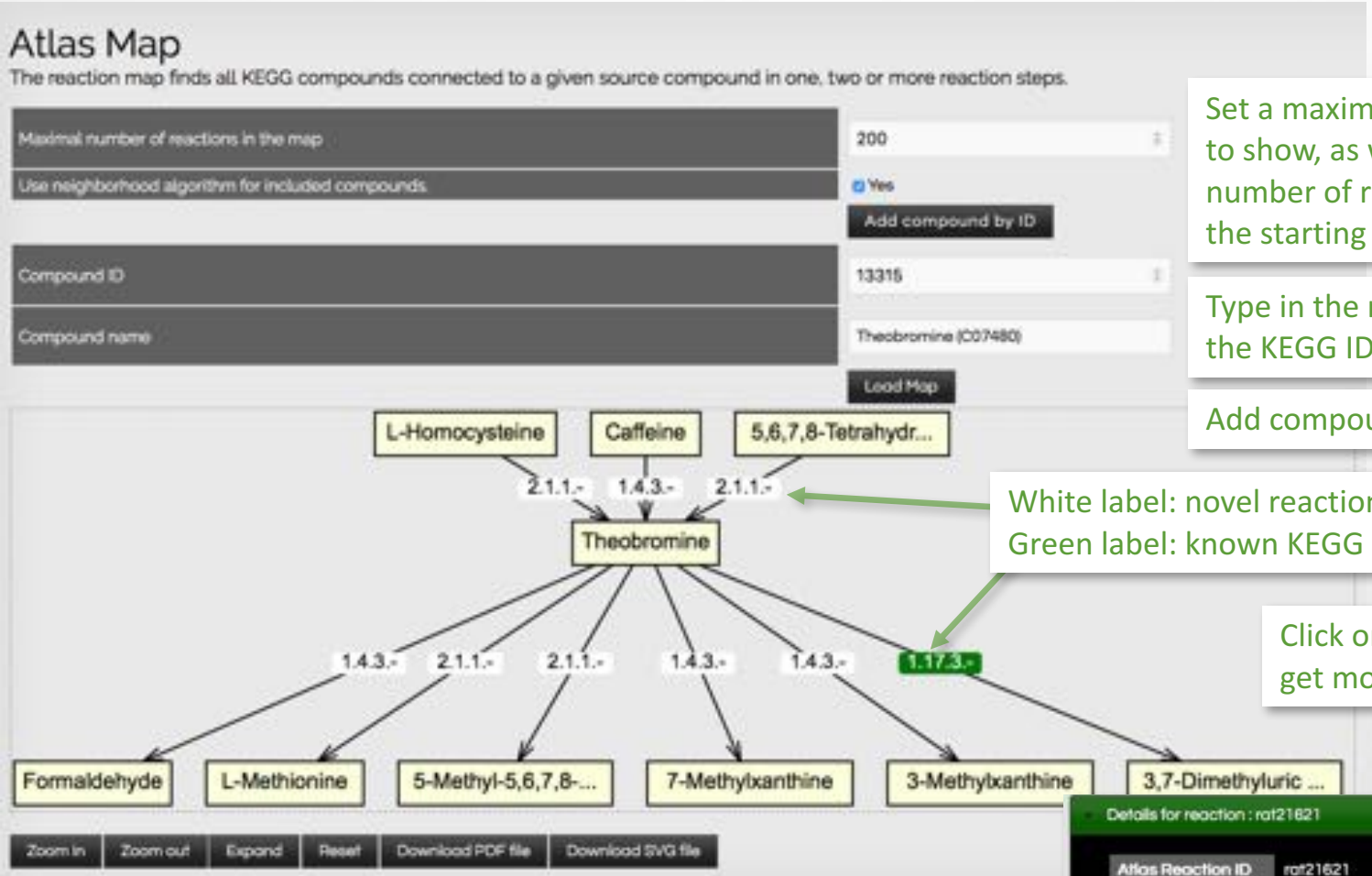
3. PATHWAYS - Graph visualization

2



4. MAPS - Metabolic environment

2



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:

Visualization settings

Download the reaction network in PDF or SVG format

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.