Rhea

Annotated reactions database

EMBL-EBI

Motivation for decomposed reactions

- The reactions provided by the NC-IUBMB are free-text...
- Can result in duplicate reactions for example....
  - acetic acid + ATP + CoA <?> acetyl-CoA + AMP

is the same as

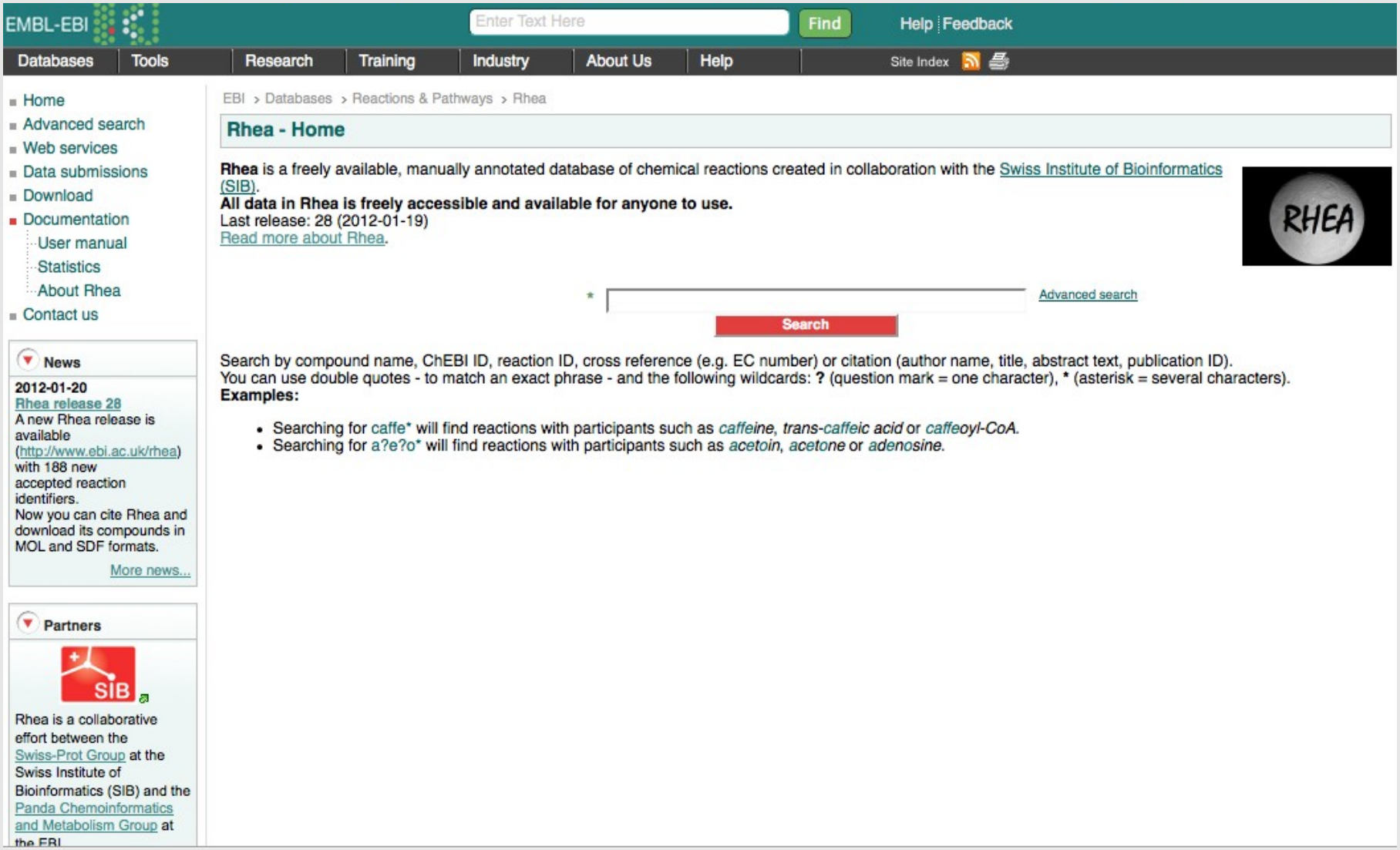
  - acetic acid + CoA + ATP <?> acetyl-CoA + AMP

But unless you tell a computer that it will just interpret two different strings....

What is Rhea

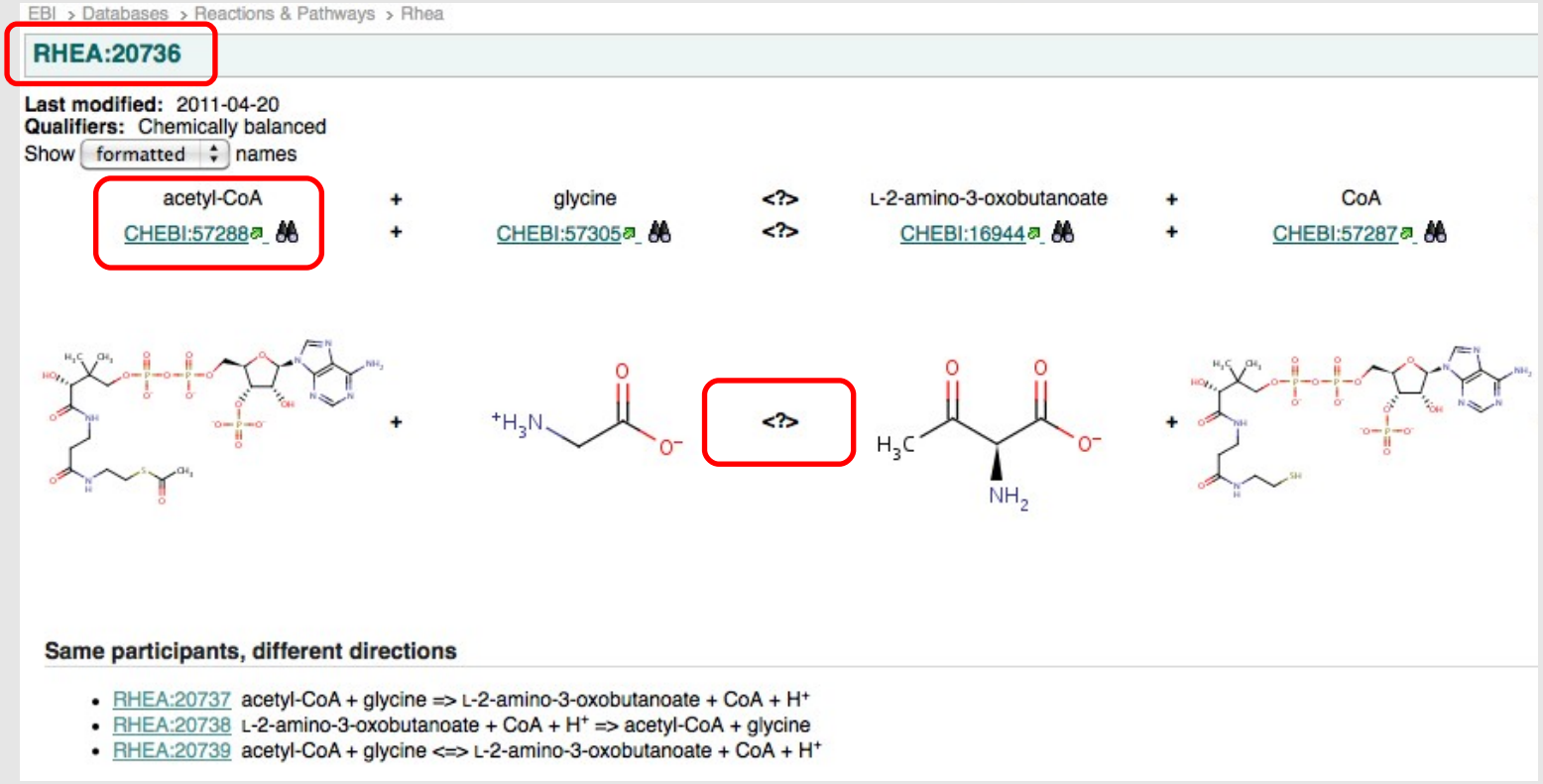
- A manually annotated database of reactions.
- Initially populated with reactions from the EC nomenclature (IntEnz/ENZYME databases).
- Also contains non-enzymatic (spontaneous) reactions of biological interest.

www.ebi.ac.uk/rhea



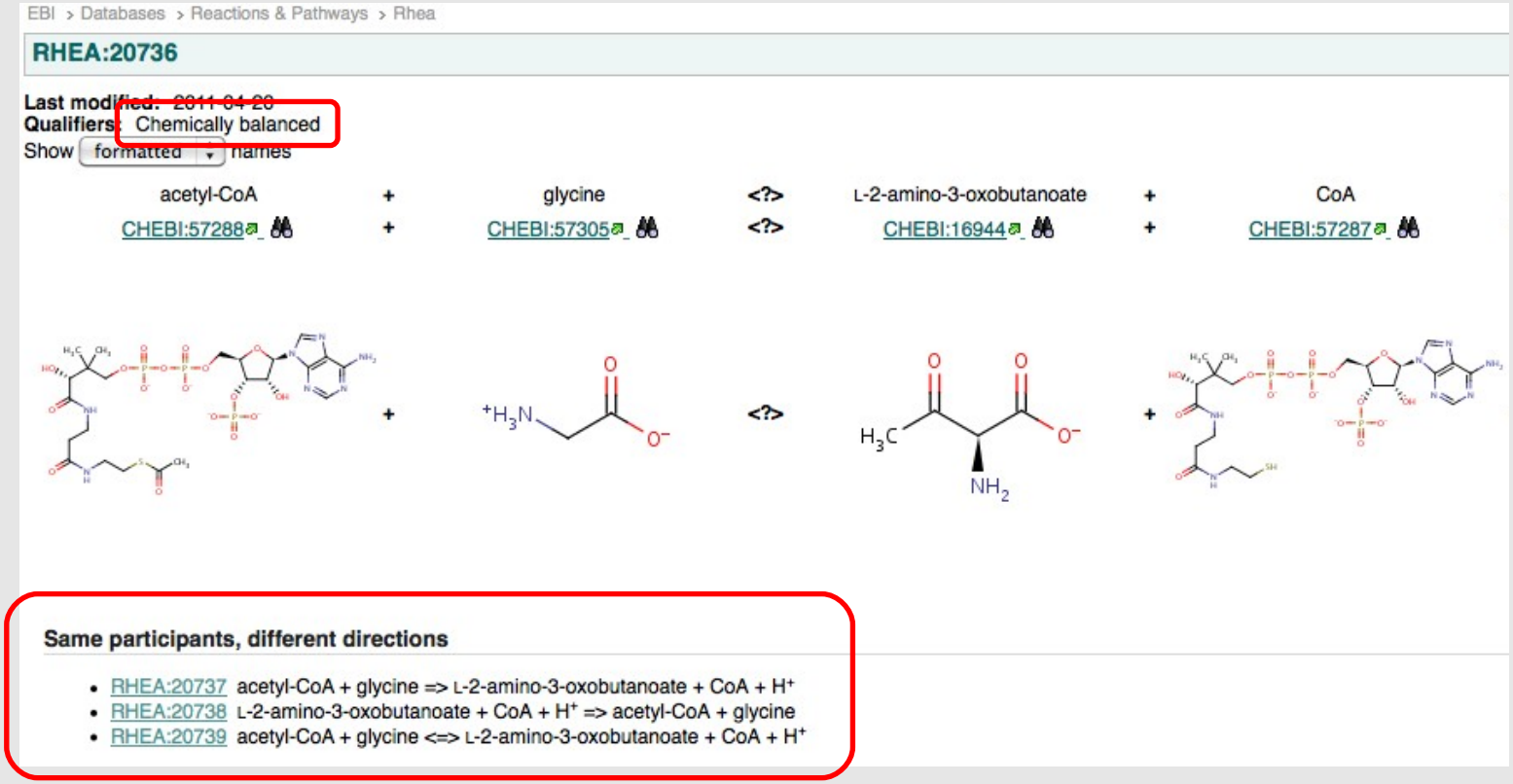
What does Rhea provide

- Stable reaction identifiers and directionality (or lack of it).
- Reaction participants linked to ChEBI



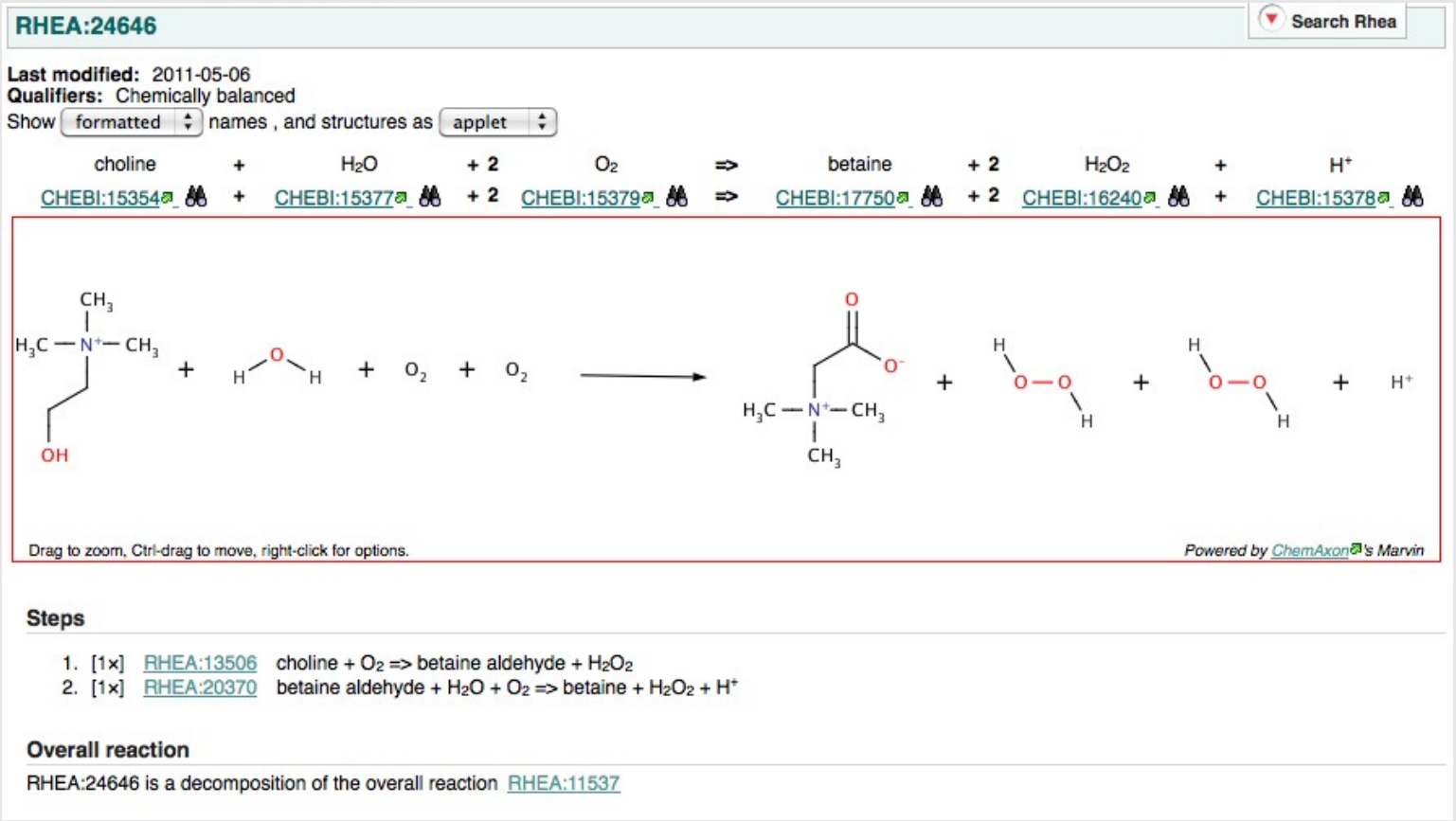
What does Rhea provide (continued)

- Validation of stoichiometry (mass and charge balance)
- Families of reactions



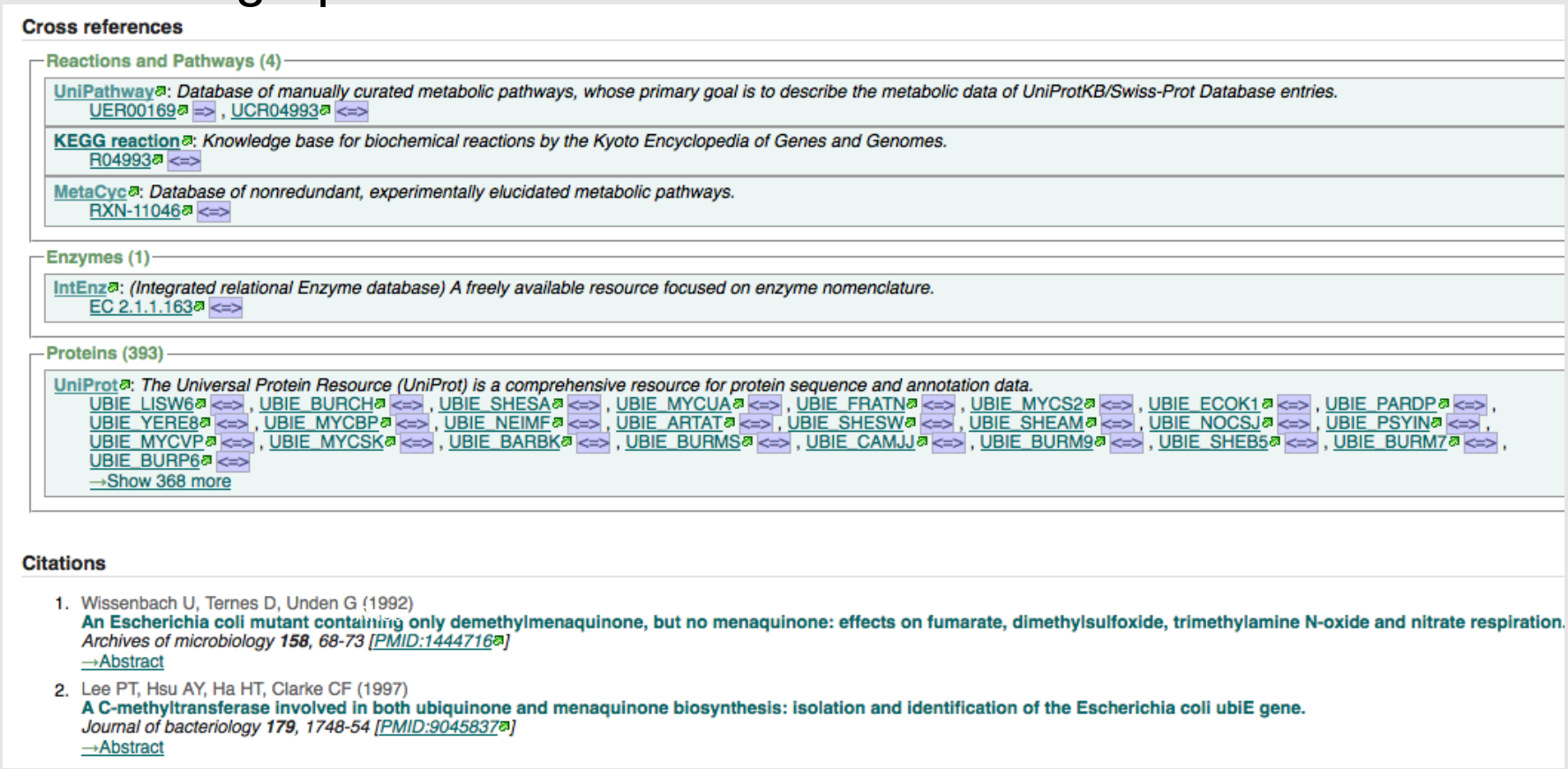
What does Rhea provide (continued)

- Decompositions of reactions in elementary processes ordered in time (steps) or not (coupled).



What does Rhea provide (continued)

- Cross references.
- Bibliographic citations.



Cross references

Reactions and Pathways (4)

UniPathway: *Database of manually curated metabolic pathways, whose primary goal is to describe the metabolic data of UniProtKB/Swiss-Prot Database entries.*
UER00169 => , UCR04993 <=>

KEGG reaction: *Knowledge base for biochemical reactions by the Kyoto Encyclopedia of Genes and Genomes.*
R04993 <=>

MetaCyc: *Database of nonredundant, experimentally elucidated metabolic pathways.*
RXN-11046 <=>

Enzymes (1)

IntEnz: *(Integrated relational Enzyme database) A freely available resource focused on enzyme nomenclature.*
EC 2.1.1.163 <=>

Proteins (393)

UniProt: *The Universal Protein Resource (UniProt) is a comprehensive resource for protein sequence and annotation data.*
UBIE_LISW6 <=> , UBIE_BURCH <=> , UBIE_SHESA <=> , UBIE_MYCUA <=> , UBIE_FRATN <=> , UBIE_MYCS2 <=> , UBIE_ECOK1 <=> , UBIE_PARDP <=> , UBIE_YERE8 <=> , UBIE_MYCBP <=> , UBIE_NEIMF <=> , UBIE_ARTAT <=> , UBIE_SHESW <=> , UBIE_SHEAM <=> , UBIE_NOCSJ <=> , UBIE_PSYIN <=> , UBIE_MYCVP <=> , UBIE_MYCSK <=> , UBIE_BARBK <=> , UBIE_BURMS <=> , UBIE_CAMJJ <=> , UBIE_BURM9 <=> , UBIE_SHEB5 <=> , UBIE_BURM7 <=> , UBIE_BURP6 <=>
→Show 368 more

Citations

1. Wissenbach U, Ternes D, Unden G (1992)
An Escherichia coli mutant containing only demethylmenaquinone, but no menaquinone: effects on fumarate, dimethylsulfoxide, trimethylamine N-oxide and nitrate respiration.
Archives of microbiology ***158***, *68-73 [PMID:1444716]*
→Abstract
2. Lee PT, Hsu AY, Ha HT, Clarke CF (1997)
A C-methyltransferase involved in both ubiquinone and menaquinone biosynthesis: isolation and identification of the Escherichia coli ubiE gene.
Journal of bacteriology ***179***, *1748-54 [PMID:9045837]*
→Abstract

Rhea compared to similar reaction DBs

- Consistency in the use of compounds and their nomenclature.
- Directionality.
- Stoichiometry check.
- Independence from spatial location.

Compounds in Rhea

- Unique name (SOURCE='UniProt' in ChEBI)

→ 'CoA'/'CoA-SH'/'Coenzyme A' problem solved.

- Normalized to pH 7.3.
- Updated with any changes in ChEBI (name, formula, merging of ChEBI ID).

Simple search

- By compound name:

  ➔urea

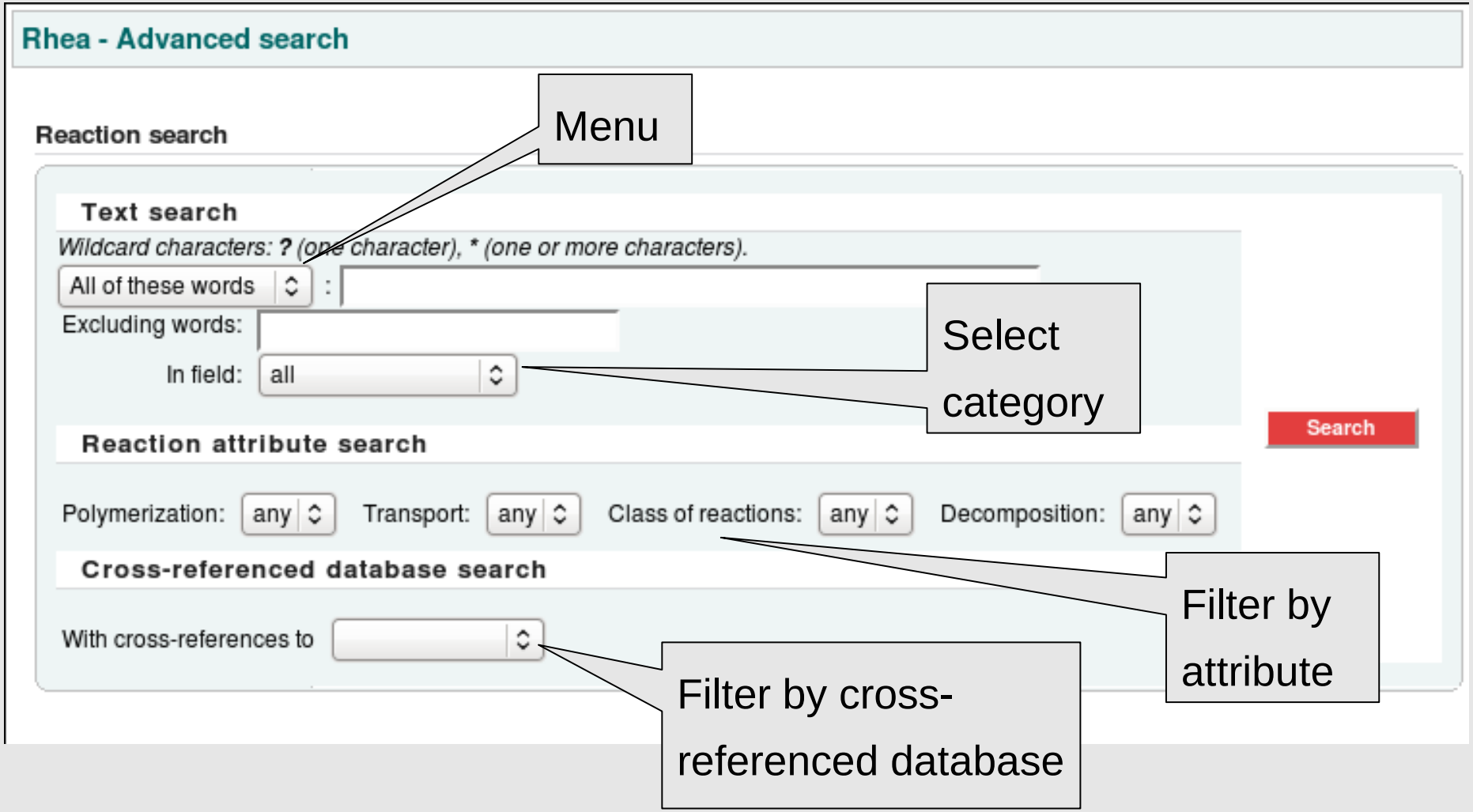
  ➔Caffe*

  ➔a?e?o*

- By compound identifier:

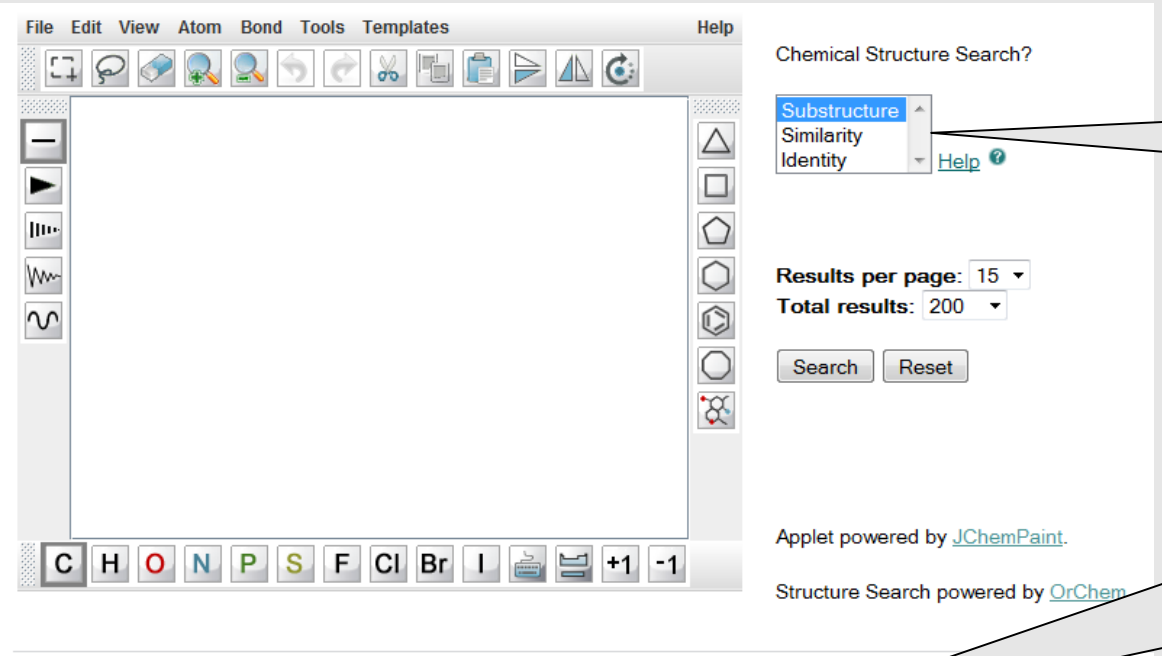
  ➔CHEBI:17015

Advanced Search - Text



EMBL-EBI

Advanced Search - Chemical



Search type

Search on formula and range searches

Rhea selected

Text Queries: (Example: water)
AND in Category All

Formula: (Example: NaHCO3) *Case sensitive.
AND Formula:

Mass range: (Example: 0 to 30.5)
AND range from to

Charge range: (Example: -1 to 1)
AND range from None to None

Filter by Ontology Term: (Example "is a CHEBI:15377" or "is a water")
AND Select relationship

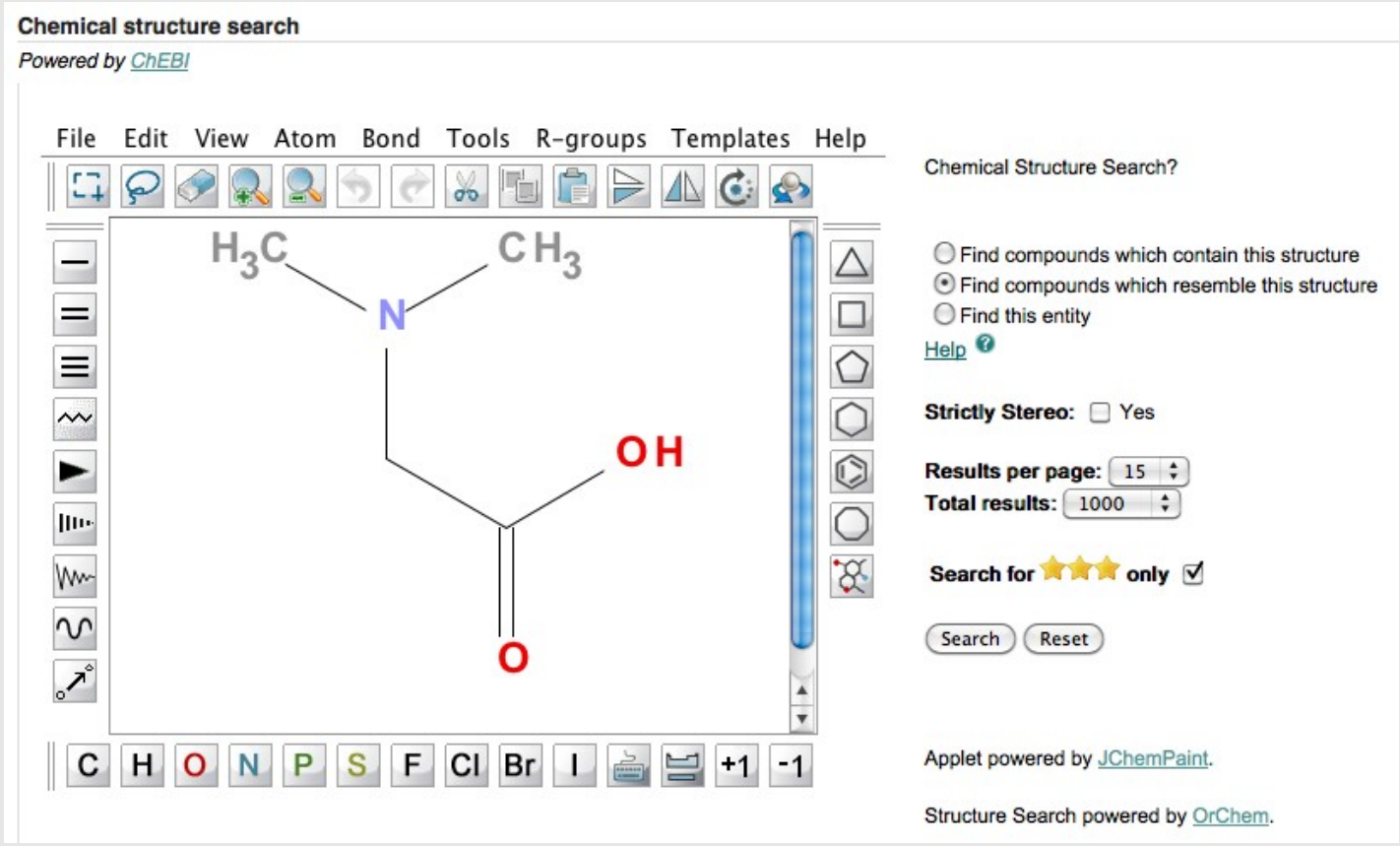
Filter by Database:
AND contains a database cross-reference in Rhea

Filter by Stars:
Results for: All Stars

Filter by Chemical Structure:
Results only with chemical structures? Yes: No:

EMBL-EBI

Advanced Search Example



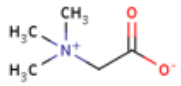
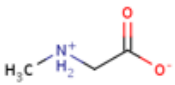
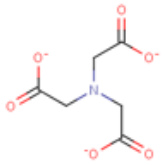
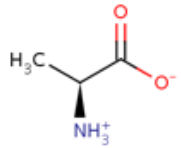
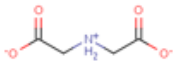
Advanced Search Example (continued)

You searched for
Rhea in Cross Reference Sources, and **3 in Stars, and structures similar to**

Edit Query

Download your search results: Tab-delimited, XML, SDF

5 entries found, displaying 1 to 5. << < 1 > >>

 CHEBI:17750 glycine betaine Stars: ★★★ Rhea reactions	 CHEBI:57433 sarcosine zwitterion Stars: ★★★ Rhea reactions	 CHEBI:25548 nitrilotriacetate(3−) Stars: ★★★ Rhea reactions
 CHEBI:57972 L-alanine zwitterion Stars: ★★★ Rhea reactions	 CHEBI:62745 ammoniodiacetate Stars: ★★★ Rhea reactions	

5 entries found, displaying 1 to 5. << < 1 > >>

Downloads

- BioPAX format (http://www.biopax.org).
- RXN format (http://www.mdl.com).
- RD format (http://www.mdl.com).
- Compounds: RD, SDF formats (http://www.mdl.com).

Web services

- http://www.ebi.ac.uk/rhea/rest/1.0/
- Simple text search
- RXN format (http://www.mdl.com).
- BioPAX level 2 format (http://www.biopax.org).
- CMLReact format.

Rhea team and resources

Rafael Alcántara (Developer, EBI)

Kristian Axelsen (Curator, SIB)

Anne Morgat (Curator, SIB)

Mohamed Zerara (Developer, SIB)

Alan Bridge (Coordinator, SIB)

Paula de Matos (Coordinator, EBI)

Christoph Steinbeck (Team leader, EBI)

http://www.ebi.ac.uk/rhea

ftp://ftp.ebi.ac.uk/pub/databases/rhea

http://sourceforge.net/projects/rhea-ebi

rhea-ebi-help@lists.sourceforge.net

EMBL-EBI

Exercises!

http://www.ebi.ac.uk/rhea