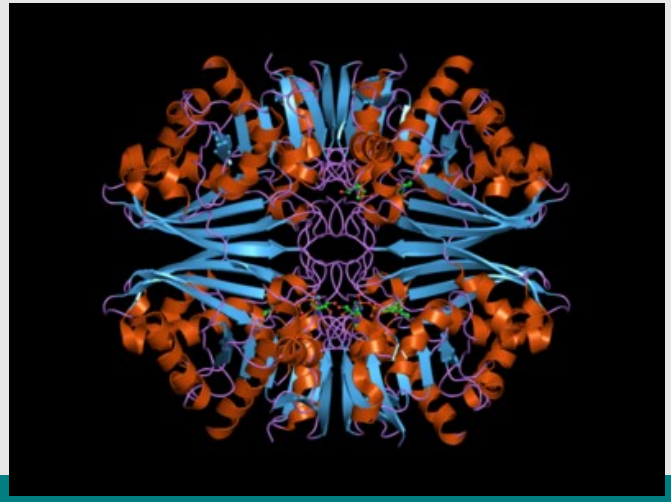
IntEnz

Integrated relational Enzyme database

EMBL-EBI

Enzymes

- Enzymes are proteins that catalyze chemical reactions.
- Very important as many processes in biological cells need enzymes....
- As there are many enzymes in the world, a classification system was invented to help identify and name them...



NC-IUBMB

- In the 1950’s the increasing amounts of known enzymes were causing confusion. No official nomenclature system for enzymes.

- The IUBMB created the International Commission on Enzymes in 1956 to deal with enzyme nomenclature

- Later replaced with the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (NC-IUBMB)

EC Numbers

- NC-IUBMB developed the Enzyme Classification number system (EC)
- Classification system is based on the reactions the enzymes catalyzed

- Classification:
  - Classes
  - Subclasses
  - Sub-subclasses
  - EC numbers (**E**nzyme **C**ommission)

- Example EC 1.1.1.1

EC Classification - Classes

EC 1 – Oxidoreductases; catalyze oxidation/reduction reactions.

EC 2 – Transferases; transfer a functional group e.g. Methyl group.

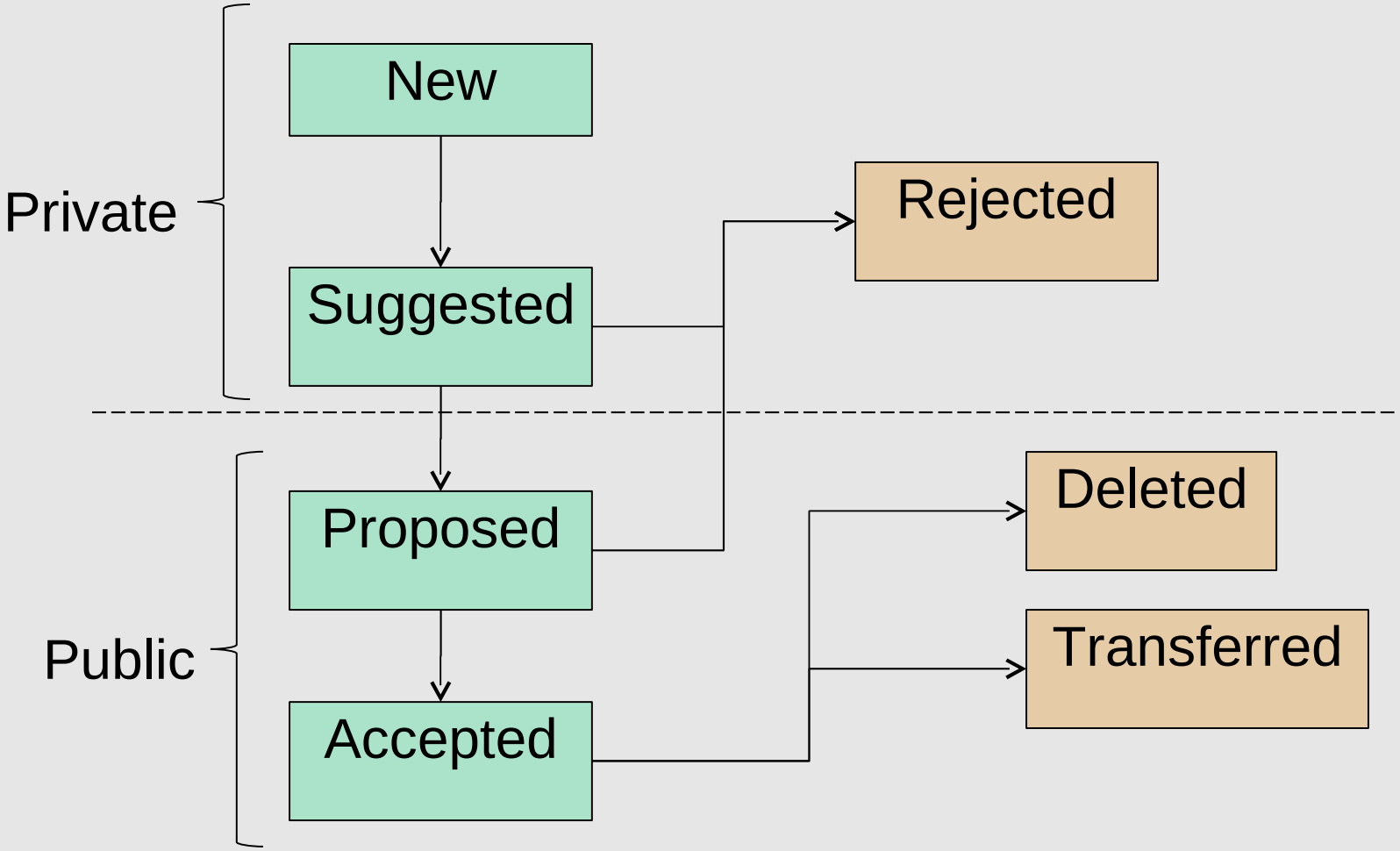
EC 3 – Hydrolases; catalyse the hydrolysis of various bonds.

EC 4 – Lyases; cleave various bonds by means other than hydrolysis and oxidation

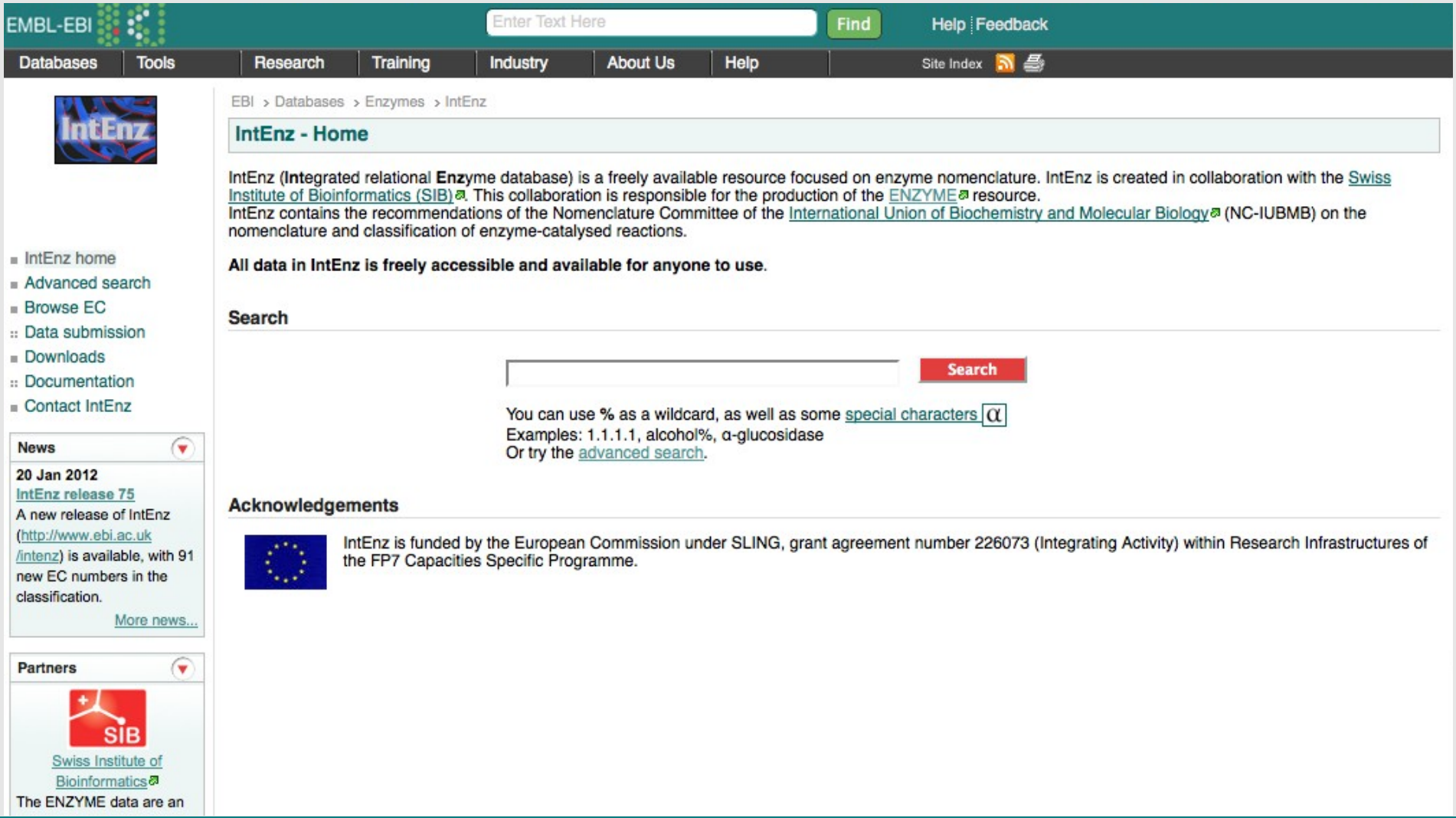
EC 5 – Isomerases; catalyse changes within one molecule.

EC 6 – Ligases; joining of two molecules with concomitant hydrolysis of the diphosphate bond in ATP or a similar triphosphate.

EC numbers lifecycle



IntEnz (www.ebi.ac.uk/intenz)



What's in IntEnz

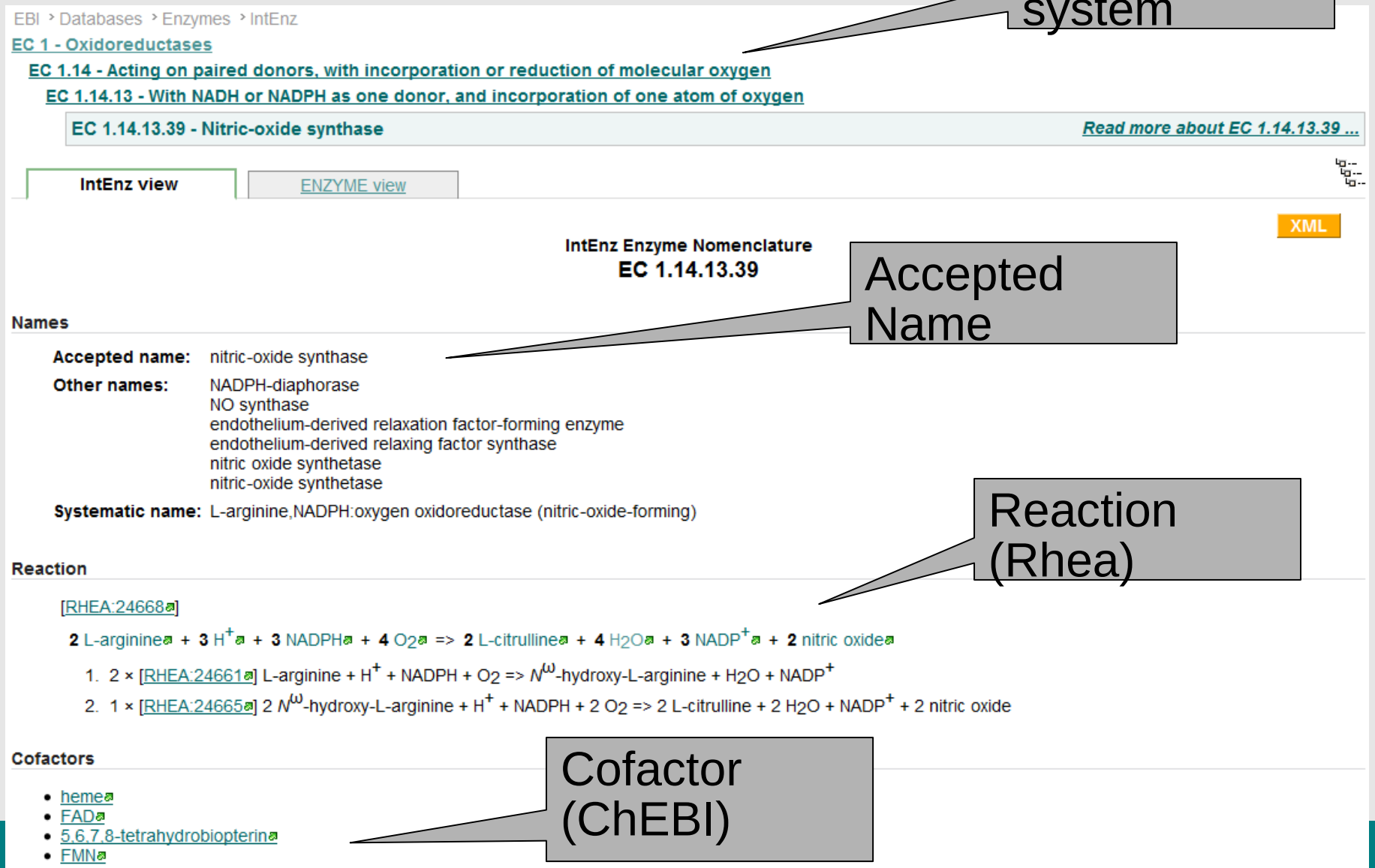
- Official Enzyme nomenclature from **NC-IUBMB**
- Data from **ENZYME** database (SIB)
  - Cofactors
  - Extra cross references: UniProtKB/Swiss-Prot, Prosite
- Extra cross references: CSA, GO
- Enzyme spotlights
- Two different views of the same data:
  - IntEnz
  - ENZYME

The (official) enzyme nomenclature

- Classification:
  - Classes
  - Subclasses
  - Sub-subclasses
  - EC numbers (**E**nzyme **C**ommission)
- Nomenclature
- Reactions (as *plain text*)
- Comments
- Cross references: BRENDA, EXPASY, KEGG, ERGO, PDB, CAS registry
- Bibliographic references

Maintained by NC-IUBMB

IntEnz Entry



IntEnz entry continued

Comments:

The enzyme in brain, but not that induced in lung or liver by endotoxin, requires Ca^{2+}. The stoichiometry is not clear, but may involve a two-electron and a one-electron oxidation step.

Links to other databases

BRENDA, CSA, ENZYME@ExPASy, GO:0004517, KEGG, NC-IUBMB, EC2PDB, CAS Registry Number: 125978-95-2

UniProtKB/Swiss-Prot: (33)
[show]

UniProt Links

References

1. Bredt, D.S. and Snyder, S.H.
   Isolation of nitric oxide synthetase, a calmodulin-requiring enzyme.
   Proc. Natl. Acad. Sci. USA **87**: 682-685 (1990). [PMID: 1689048]
2. Knowles, R.G., Merrett, M., Salter, M. and Moncada, S.
   Differential induction of brain, lung and liver nitric oxide synthase by endotoxin in the rat.
   Biochem. J. **270**: 833-836 (1990). [PMID: 1700698]
3. Moncada, S., Palmer, R.M.J. and Higgs, E.A.
   Biosynthesis of nitric oxide from L-arginine. A pathway for the regulation of cell function and communication.
   Biochem. Pharmacol. **38**: 1709-1715 (1989). [PMID: 2567594]

Citations

[EC 1.14.13.39 created 1992]

Simple search

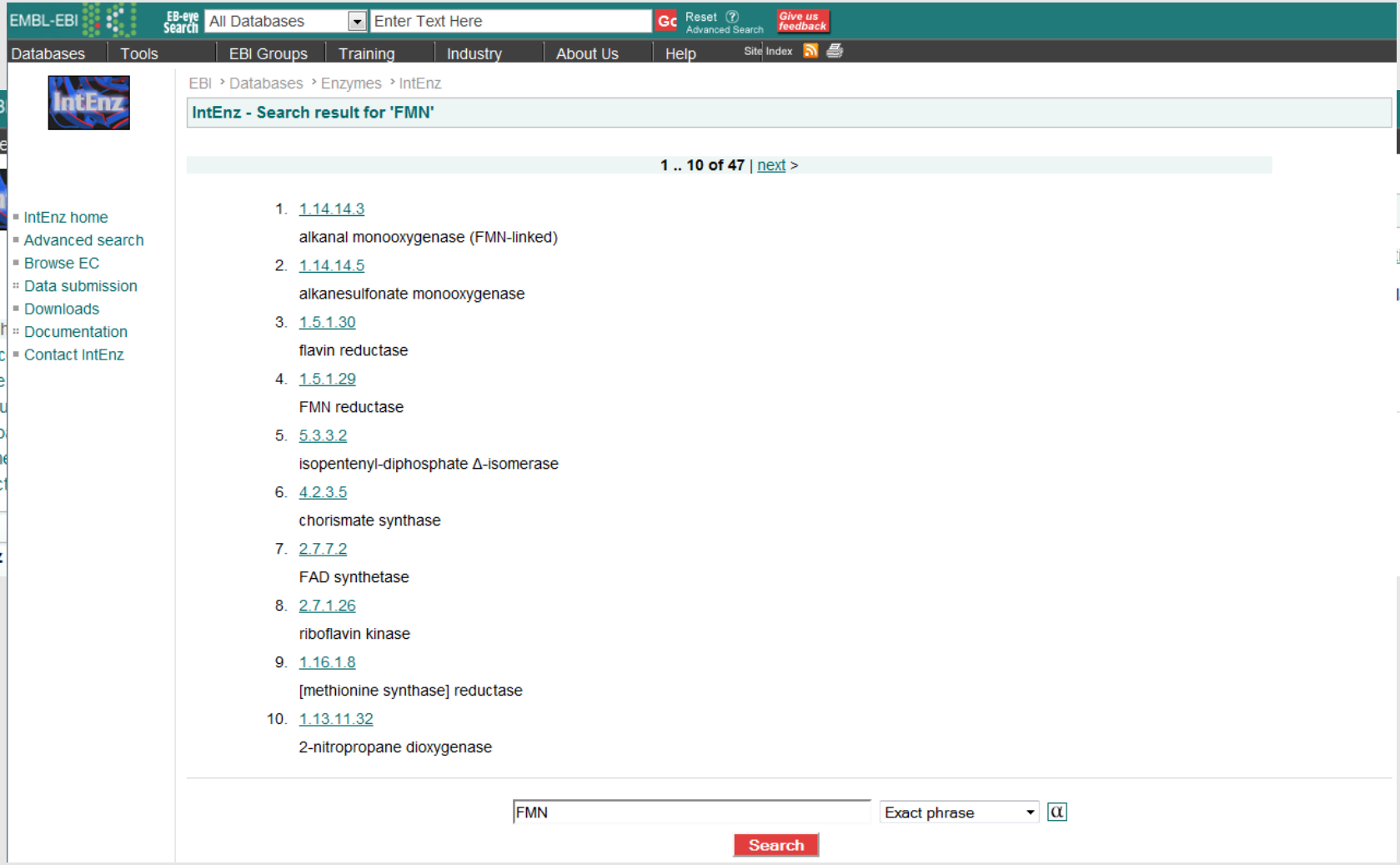
- Search by EC number:
  - 1.1.1.1
  - 1.2.3.12
  - 1.13.1.13

- Search by enzyme name:
  - ➔Oxalate oxidase
  - ➔Agarase
  - ➔3/4 collagenase

- Search by cross-reference:
  - ➔Q42884
  - ➔GO:0047948

- Search by compound:
  - ➔Caffeine
  - ➔CoA

Simple Search Example

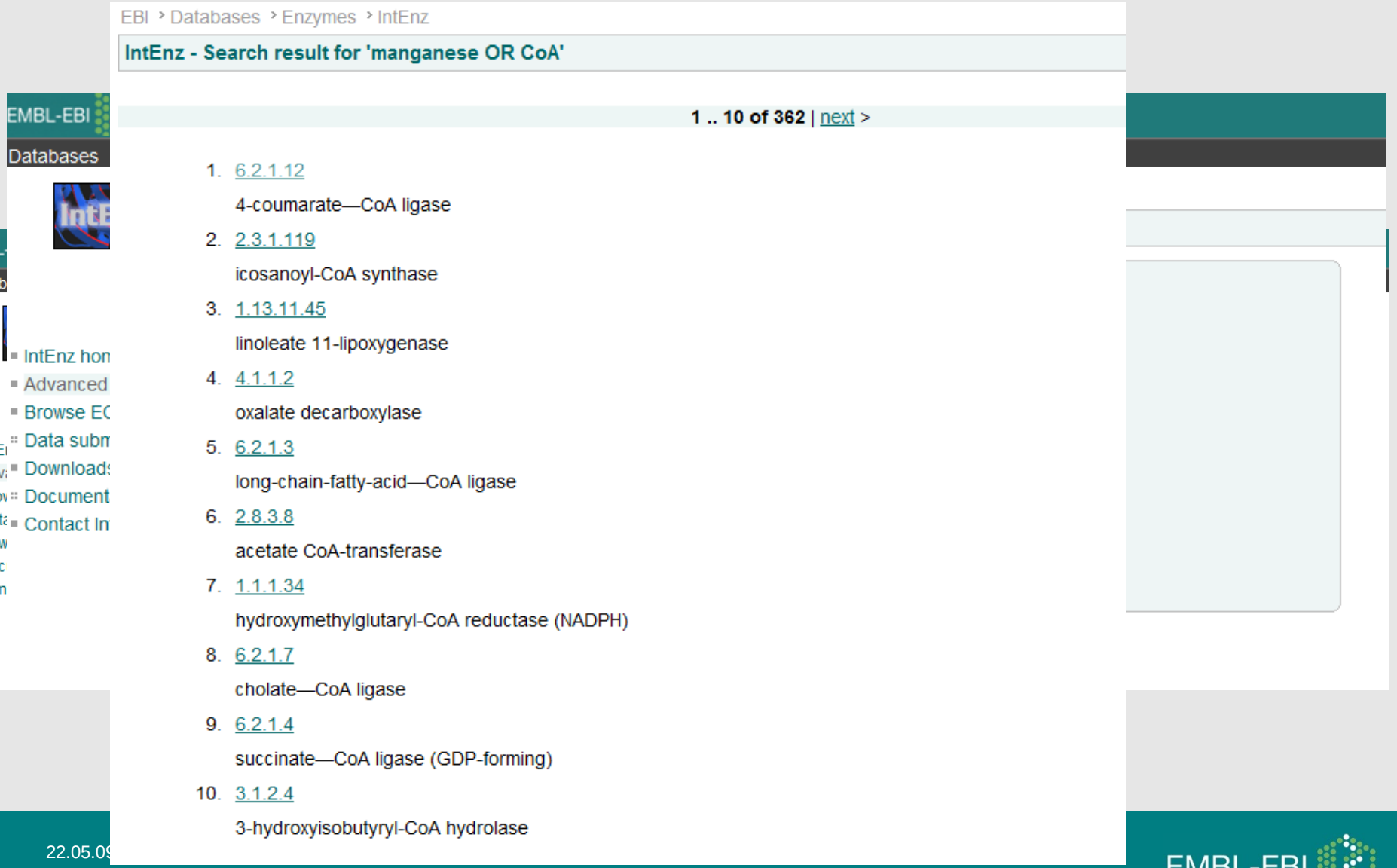


Advanced search

- Search by reaction participant:
  - CoA
  - CoA-SH
  - CoASH
  - Coenzyme-A

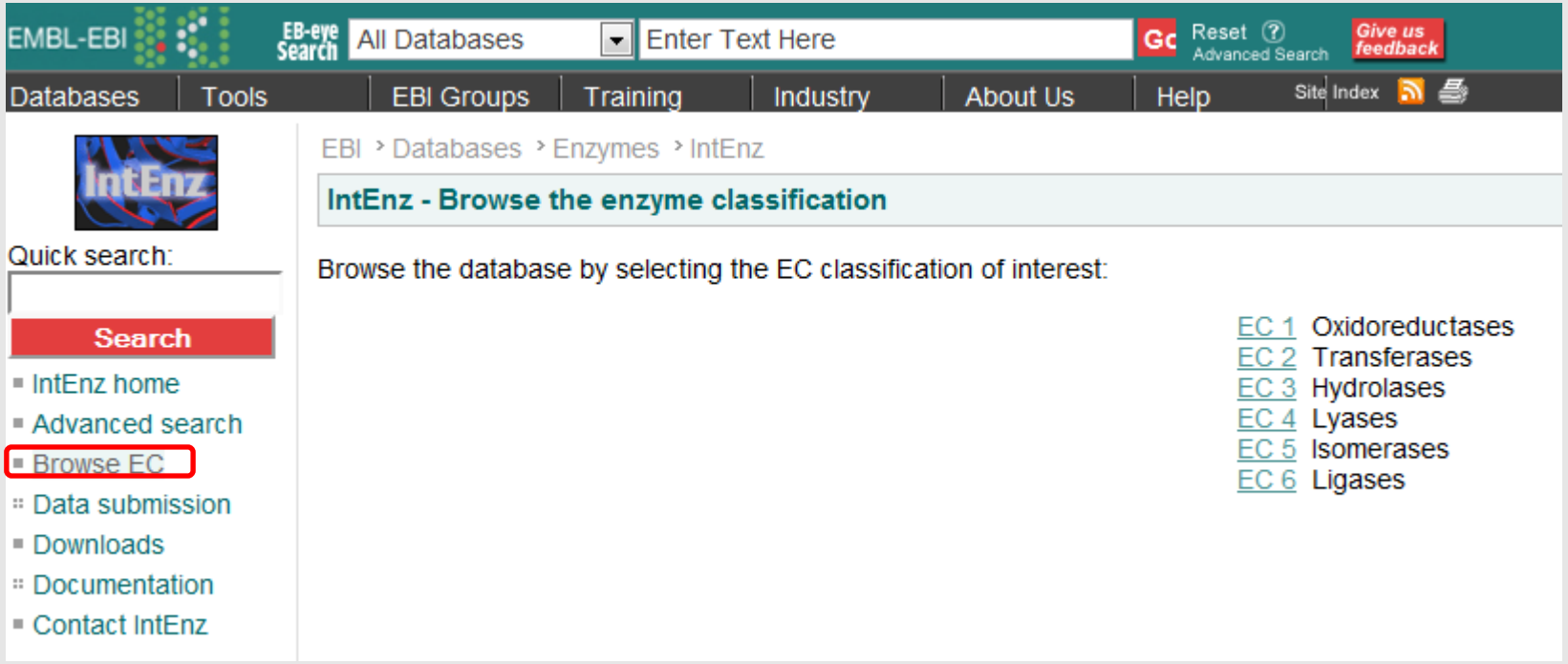
- Search by cofactor:
  - ➔CoA
  - ➔magnesium manganese (any)
  - ➔magnesium manganese (both)

Advanced Search Example



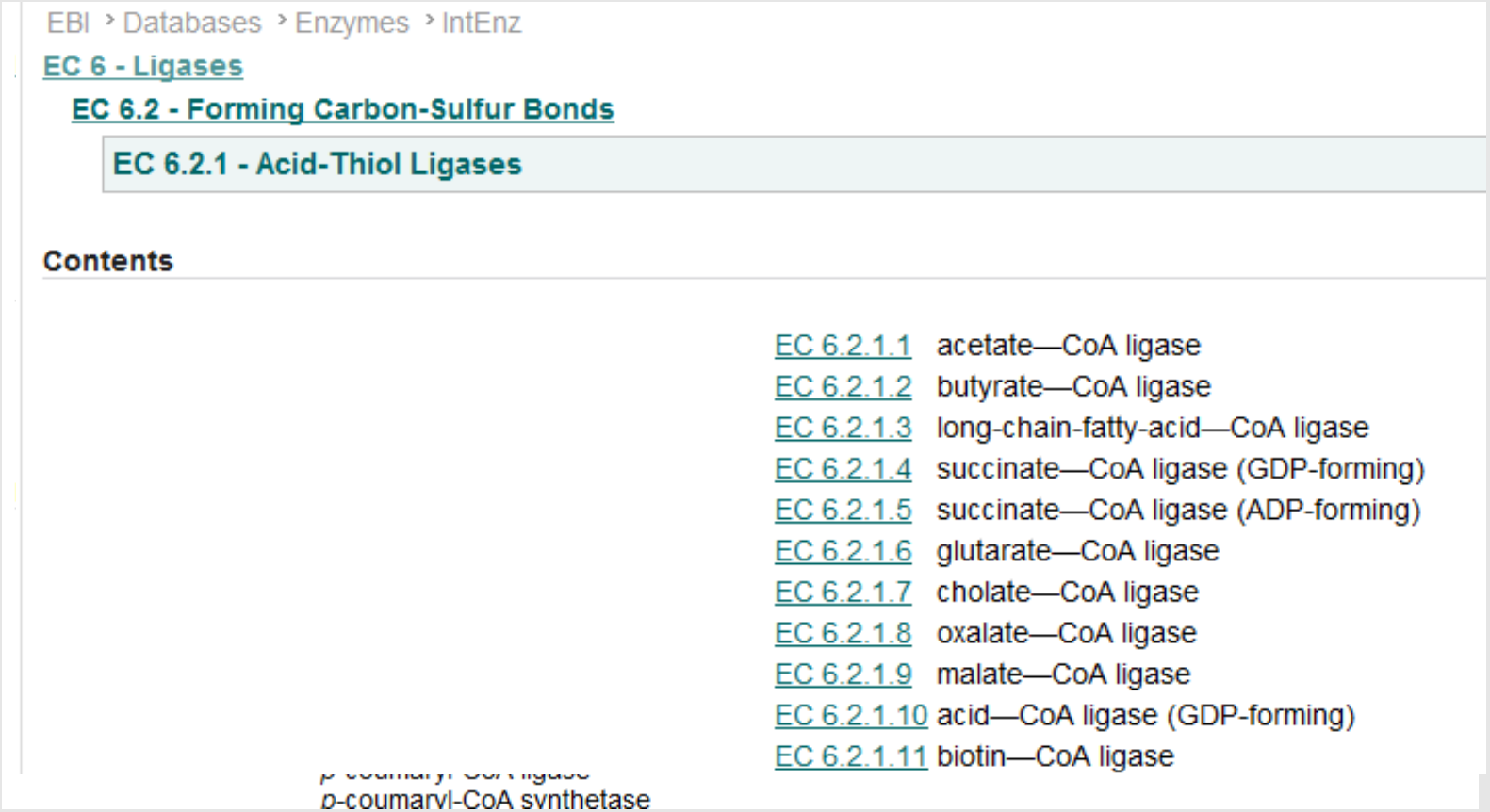
Browsing IntEnz

- Browse the whole classification from the home page



Browsing via Enzyme entry

- Browse upwards from an enzyme entry



Downloading IntEnz

- **IntEnzXML**
  - Individual enzymes/all of them
  - ASCII format/XChars-enhanced format
  - XSD available
  - Query/format using XSLT

- **enzyme.dat** file
  - Generated from IntEnz for SIB

- **BioPAX level 2**
  - A standard exchange format for biological pathway data
  - Based in OWL (semantic web)

IntEnz team and resources

Rafael Alcántara (Developer, EBI)
Kristian Axelsen (Curator, SIB)
Paula de Matos (Coordinator, EBI)
Anne Morgat (Curator, SIB)
Christoph Steinbeck (Team leader, EBI)

http://www.ebi.ac.uk/intenz
ftp://ftp.ebi.ac.uk/pub/databases/intenz
http://sourceforge.net/projects/intenz
intenz-help@lists.sourceforge.net

EMBL-EBI

Exercises!

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