ChemTunes Metabolism Database

Exogenous and Endogenous Metabolic Pathways

ChemTunes Metabolism Database is a database of biotransformations of chemical compounds that covers both the exogenous and the endogenous metabolism.

The data on exogenous metabolism (xenobiotics) includes human hepatic transformations of drugs and drug-like molecules collected from the literature as well as *in vivo/in vitro* metabolic studies in laboratory and farm animals and primates for pesticides collected from EFSA opinions.

The data on the endogenous metabolism provides access to metabolic transformations and cellular regulations derived from the "Biochemical Pathways" wall chart and additional harvesting of literature data.

Features

- Unique combination of toxicity data (ChemTunes Toxicity Database) and information about metabolic transformations
- Manually quality-controlled by domain experts
- Exogenous metabolism
  - *Information about parent/metabolite relationship*
  - *Classification into major and minor metabolites*
  - *Up to five levels of metabolic degradation*
- Endogenous metabolism
  - *Information on enzymes (name and EC) and pathways (names)*
- Molecules stored with connection tables including stereochemical information

Key Facts

Exogenous metabolism

- *Drugs, pesticides, and industrial chemicals*
- *Over 5,500 chemical structures with 500 parents and over 5,000 metabolites*
- *Over 2,800 chemical reactions*
- *Over 140 reaction types*

Endogenous metabolism

- ***Four species:** prokaryotes, animals, plants and yeasts, and general*
- *Over 2,700 chemical structures*
- *Over 3,900 chemical reactions*
- *Total of 640 pathways*

Areas of Application

- Identification of metabolism-meditated toxicity
- Verification of predicted transformations of xenobiotics by **ChemTunes Metabolizer**
- Support of New Approach Methodologies (NAM) and Next Generation Risk Assessment (NGRA) for chemical safety assessment

MN AM

Molecular Networks & Altamira
Molecular Networks GmbH, Neumeyerstraße 22-34, 90411 Nuremberg, Germany
Altamira LLC, 470 W Broad St, Unit 5007, OH 43215, USA

+49 (0)911 597 424 00
www.mn-am.com
info@mn-am.com