# BHARATHIDASAN UNIVERSITY

Tiruchirappalli- 620024,
Tamil Nadu, India.

## Programme : M.Sc., Biomedical Science

**Course Title : Bioinformatics**
**Course Code : BM35S1BI**

## Unit-II

# TOPIC: Metabolic Pathways and Enzymatic Database

**Dr. P. JEGANATHAN**
Guest Lecturer
Department of Biomedical Science

# METABOLIC PATHWAYS

# AND

# ENZYMATIC DATABASE

# CONTENTS

- ✓BIOLOGICAL PATHWAY
- ✓TYPES OF BIOLOGICAL PATHWAY
- ✓PATHWAY DATABASES
- ✓KEGG PATHWAY
- ✓19 KEGG DATABASES
- ✓ROLE OF KEGG DATABASE
- ✓METACYC
- ✓ROLE OF META CYC

# BIOLOGICAL PATHWAY

A Series of actions among molecules in a cell that leads to a certain product or change in a cell.

# TYPES OF BIOLOGICAL PATHWAY

- METABOLIC PATHWAY
- GENE REGULATION PATHWAYS
- SIGNAL TRANSDUCTION

# DATABASES

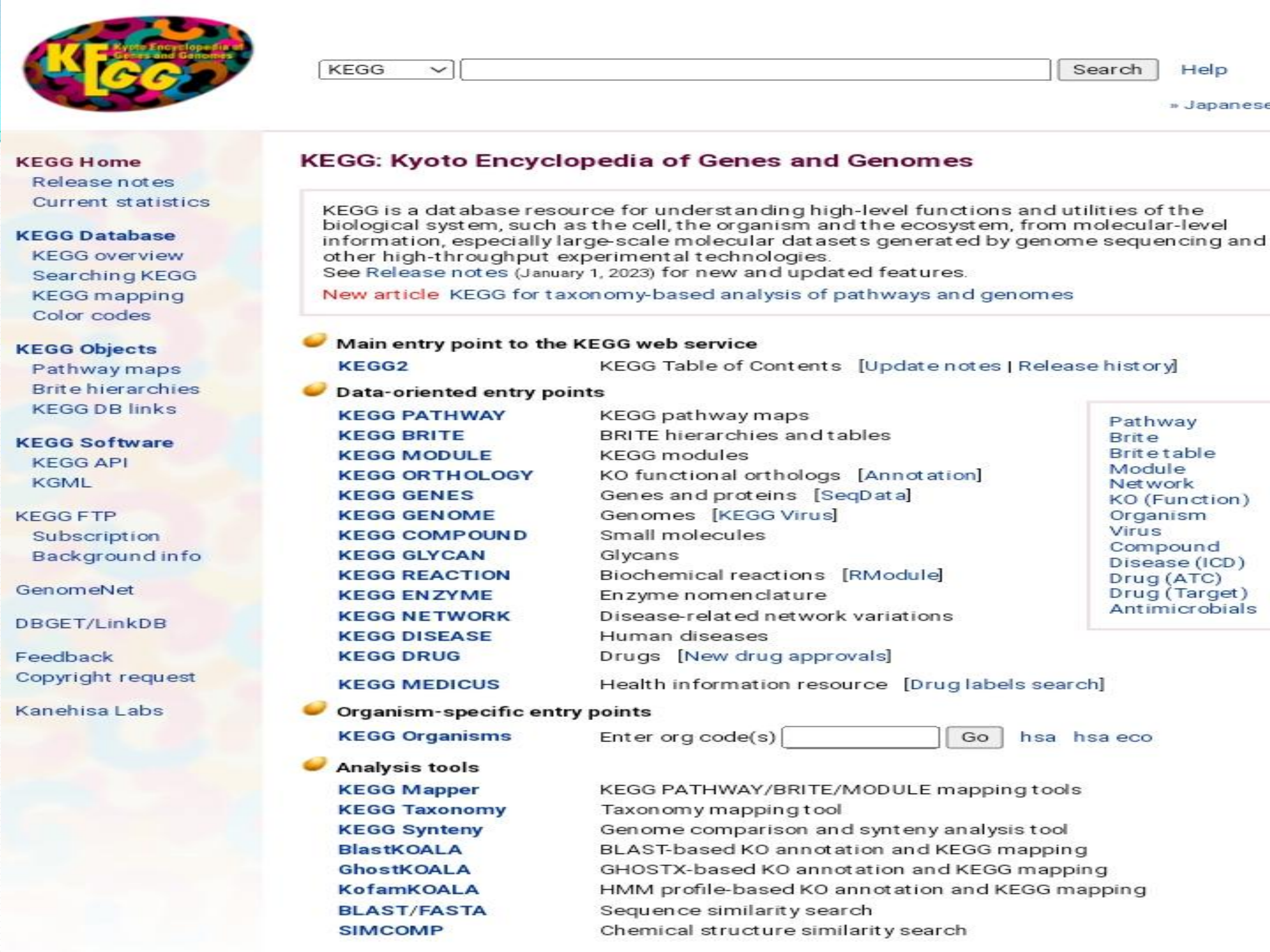
A Database is a systemic collection of data. They support electronic storage and manipulation of Data .It makes the data management easy.

# PATHWAY DATABASES

- ☐KEGG Pathway
- ☐BIOCARTA
- ☐BIOCYC
- ☐METACYC
- ☐BRENDA

# KEGG PATHWAY

KEGG(Kyoto Encyclopedia Of Genes and Genomes) is a series of databases developed by bioinformatics centre of kyoto and Human Genome Centre of the Tokyo.



KEGG Home
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KEGG Database
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Kanehisa Labs

# KEGG: Kyoto Encyclopedia of Genes and Genomes

KEGG is a database resource for understanding high-level functions and utilities of the biological system, such as the cell, the organism and the ecosystem, from molecular-level information, especially large-scale molecular datasets generated by genome sequencing and other high-throughput experimental technologies.
See Release notes (January 1, 2023) for new and updated features.

New article KEGG for taxonomy-based analysis of pathways and genomes

**Main entry point to the KEGG web service**

| | |
|---|---|
| **KEGG2** | KEGG Table of Contents [Update notes \| Release history] |

**Data-oriented entry points**

| | |
|---|---|
| **KEGG PATHWAY** | KEGG pathway maps |
| **KEGG BRITE** | BRITE hierarchies and tables |
| **KEGG MODULE** | KEGG modules |
| **KEGG ORTHOLOGY** | KO functional orthologs [Annotation] |
| **KEGG GENES** | Genes and proteins [SeqData] |
| **KEGG GENOME** | Genomes [KEGG Virus] |
| **KEGG COMPOUND** | Small molecules |
| **KEGG GLYCAN** | Glycans |
| **KEGG REACTION** | Biochemical reactions [RModule] |
| **KEGG ENZYME** | Enzyme nomenclature |
| **KEGG NETWORK** | Disease-related network variations |
| **KEGG DISEASE** | Human diseases |
| **KEGG DRUG** | Drugs [New drug approvals] |
| **KEGG MEDICUS** | Health information resource [Drug labels search] |

Pathway
Brite
Brite table
Module
Network
KO (Function)
Organism
Virus
Compound
Disease (ICD)
Drug (ATC)
Drug (Target)
Antimicrobials

**Organism-specific entry points**

| | |
|---|---|
| **KEGG Organisms** | Enter org code(s) Go hsa hsa eco |

**Analysis tools**

| | |
|---|---|
| **KEGG Mapper** | KEGG PATHWAY/BRITE/MODULE mapping tools |
| **KEGG Taxonomy** | Taxonomy mapping tool |
| **KEGG Synteny** | Genome comparison and synteny analysis tool |
| **BlastKOALA** | BLAST-based KO annotation and KEGG mapping |
| **GhostKOALA** | GHOSTX-based KO annotation and KEGG mapping |
| **KofamKOALA** | HMM profile-based KO annotation and KEGG mapping |
| **BLAST/FASTA** | Sequence similarity search |
| **SIMCOMP** | Chemical structure similarity search |

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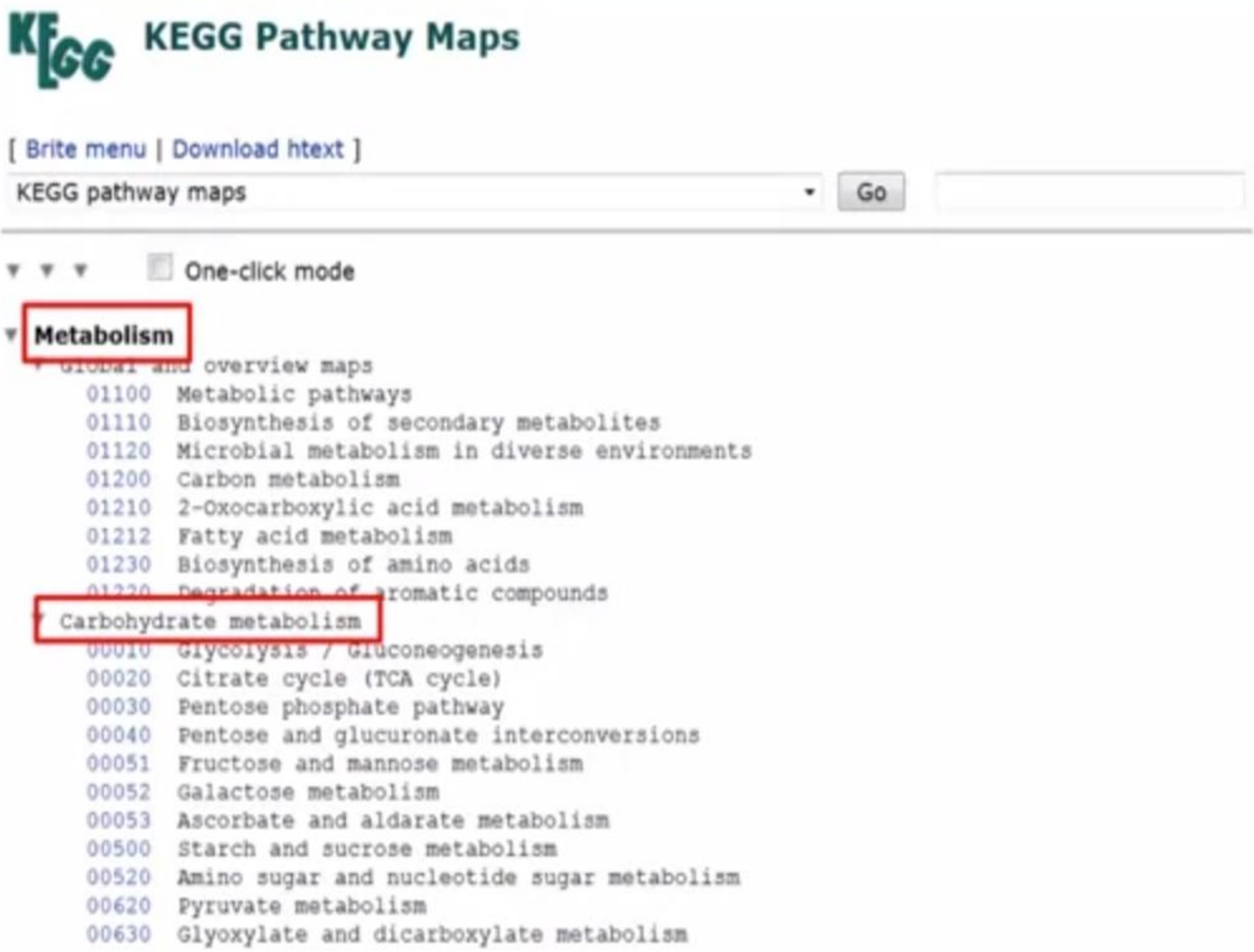
**KEGG Pathway Maps**

[ Brite menu | Download htext ]

KEGG pathway maps

▼ ▼ ▼ ☐ One-click mode

- ▶ **Metabolism**
- ▶ **Genetic Information Processing**
- ▶ **Environmental Information Processing**
- ▶ **Cellular Processes**
- ▶ **Organismal Systems**
- ▶ **Human Diseases**
- ▶ **Drug Development**



- **Metabolism**
  - Global and overview maps
    - 01100 Metabolic pathways
    - 01110 Biosynthesis of secondary metabolites
    - 01120 Microbial metabolism in diverse environments
    - 01200 Carbon metabolism
    - 01210 2-Oxocarboxylic acid metabolism
    - 01212 Fatty acid metabolism
    - 01230 Biosynthesis of amino acids
    - 01220 Degradation of aromatic compounds
  - Carbohydrate metabolism
    - 00010 Glycolysis / Gluconeogenesis
    - 00020 Citrate cycle (TCA cycle)
    - 00030 Pentose phosphate pathway
    - 00040 Pentose and glucuronate interconversions
    - 00051 Fructose and mannose metabolism
    - 00052 Galactose metabolism
    - 00053 Ascorbate and aldarate metabolism
    - 00500 Starch and sucrose metabolism
    - 00520 Amino sugar and nucleotide sugar metabolism
    - 00620 Pyruvate metabolism
    - 00630 Glyoxylate and dicarboxylate metabolism

- KEGG database has been available for over 10 years.

- The “PATHWAY” section of KEGG consists mainly of

Metabolic pathways.

- URL:http ://www.genome.jp/kegg/

- KEGG is a collection of biological information compiled from Published material.

- Includes information on genes ,proteins, metabolic Pathways, molecular interactions and biochemical reactions associated with specific organisms.

- Provides a relationship (map) for how these Components are organized in cellular structure or reaction pathways.

- *ADVANTAGE:* Information is reliable
- *DISADVANTAGE:* Information is not available for many organisms.

# 19 KEGG DATABASES

## SYSTEM INFORMTION(6)

- **PATHWAY,MODULE:** Network information
- **BRITE:** Hiearchical classification
- **DISEASE,DRUG,EDRUG**: Medical and pharmaceutical information.

# GENOMIC INFORMATION(7)

- **ORTHOLOGY:** Orthology for functional annotation
- **GENOMES:** Entrance of all information for each species
- **GENES,DGENES:** Genes for complete and draft genes
- **SSDB:** All to all genes sequences score and best hit information
- **EGENES,MGENES:** Genes for EST assemblies and meta genomes

# CHEMICAL INFORMATION(6)

- **COMPOUND:** Chemical compounds in metabolic pathways
- **GLYCAN:** Carbohydrate structures
- **REACTION:** Chemical reaction in metabolic pathway
- **REPAIR,RCLASS:** Reactant pairs and patterns from reaction
- **ENZYME:** IUPAC Enzyme nomenclature

# ROLE OF KEGG DATABASE

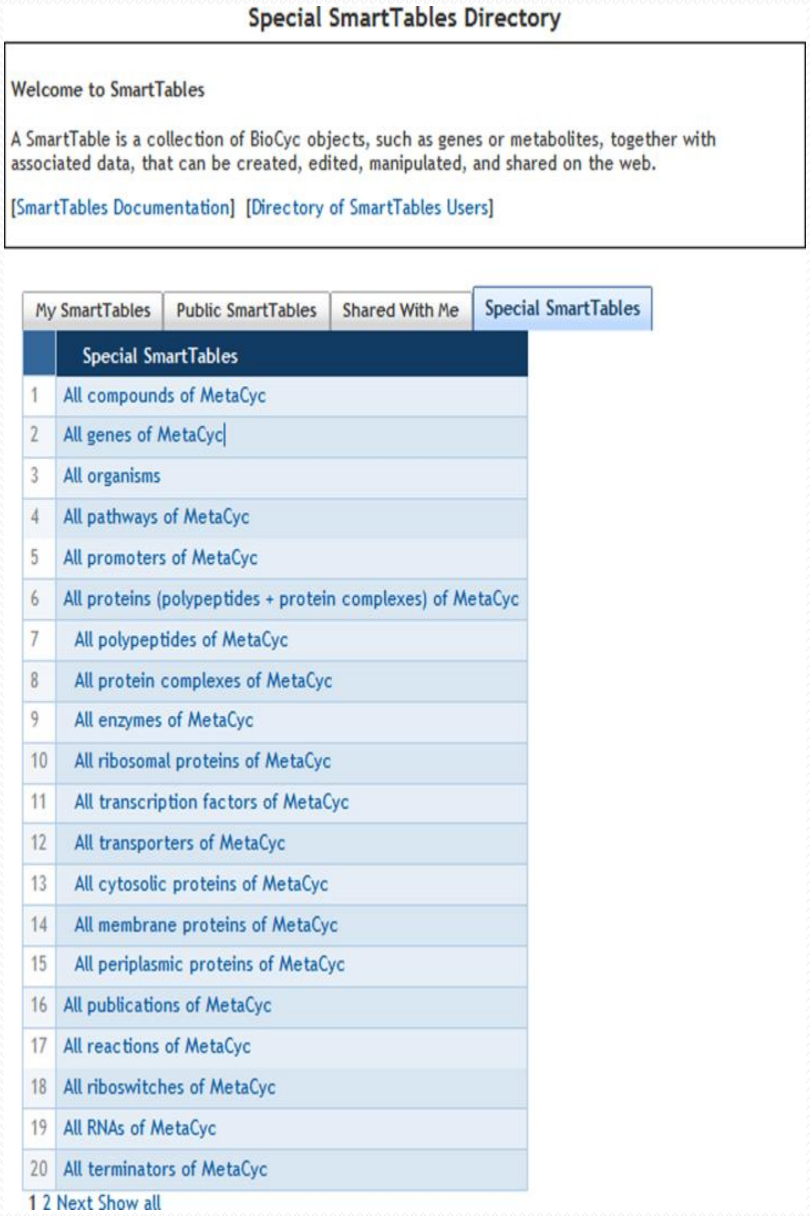
- The set of chemical reactions (metabolism) that happen in living organisms. These processes allow organism to grow, reproduce, respond to environment.
- Genetic information processing, such as DNA replication.
- Environmental information processing, such as signaling molecules and interactions.
- Cellular process like growth and death of cells.

# META CYC

- Database of non redundant, experimentally elucidated metabolic pathways.
- Contains more than **1,100** pathways from more than **1,500** different organisms.
- Contains pathway involved in both primary and secondary metabolism as well as associated compounds ,enzymes and genes.

Current Database: *MetaCyc*

Search in Current Database: Enter a gene, protein, metabolite or pathway...

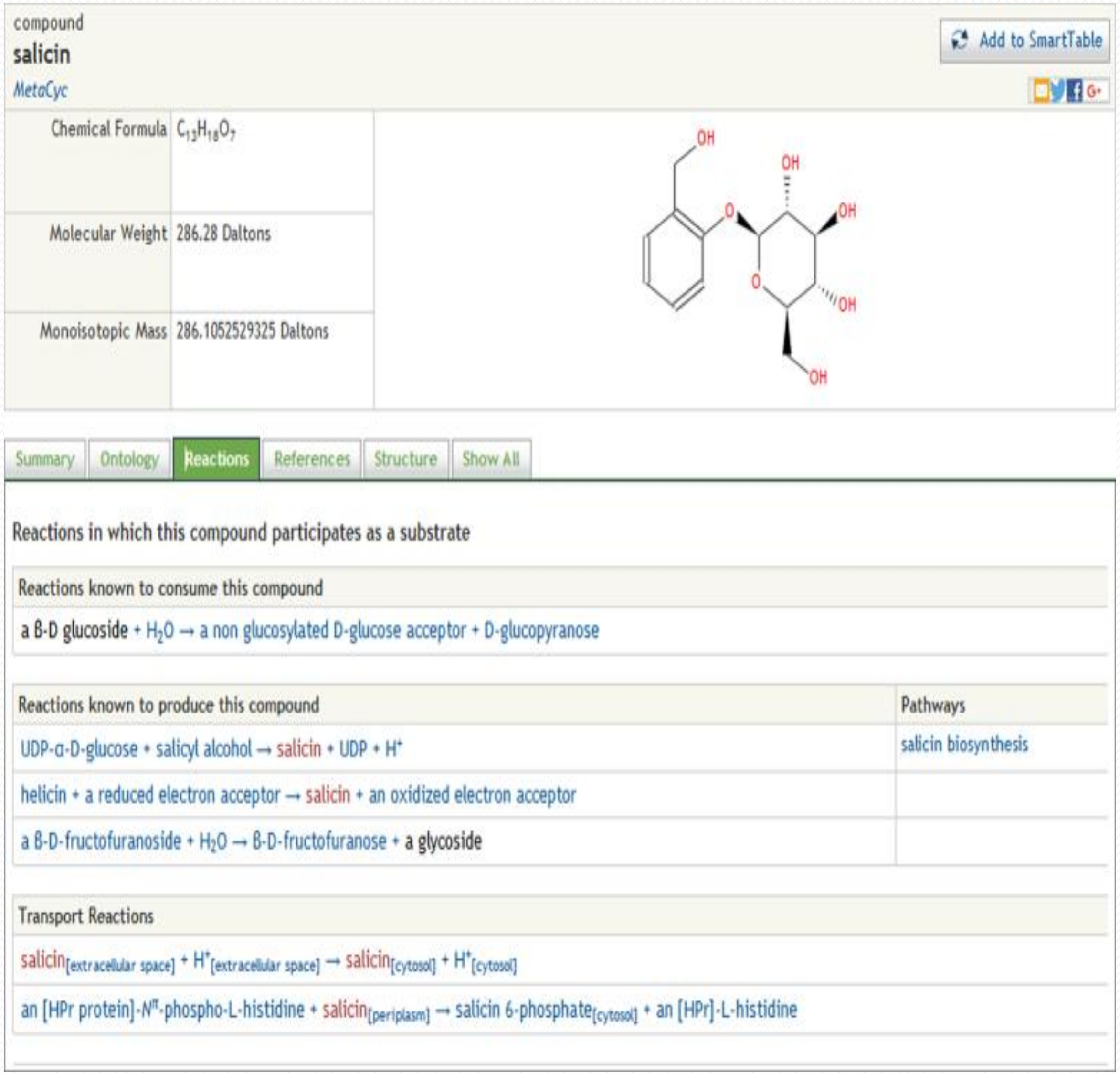

Special SmartTables Directory

Welcome to SmartTables

A SmartTable is a collection of BioCyc objects, such as genes or metabolites, together with associated data, that can be created, edited, manipulated, and shared on the web.

[SmartTables Documentation] [Directory of SmartTables Users]

| | Special SmartTables |
|---|---|
| 1 | All compounds of MetaCyc |
| 2 | All genes of MetaCyc |
| 3 | All organisms |
| 4 | All pathways of MetaCyc |
| 5 | All promoters of MetaCyc |
| 6 | All proteins (polypeptides + protein complexes) of MetaCyc |
| 7 | All polypeptides of MetaCyc |
| 8 | All protein complexes of MetaCyc |
| 9 | All enzymes of MetaCyc |
| 10 | All ribosomal proteins of MetaCyc |
| 11 | All transcription factors of MetaCyc |
| 12 | All transporters of MetaCyc |
| 13 | All cytosolic proteins of MetaCyc |
| 14 | All membrane proteins of MetaCyc |
| 15 | All periplasmic proteins of MetaCyc |
| 16 | All publications of MetaCyc |
| 17 | All reactions of MetaCyc |
| 18 | All riboswitches of MetaCyc |
| 19 | All RNAs of MetaCyc |
| 20 | All terminators of MetaCyc |



compound

**salicin**

*MetaCyc*

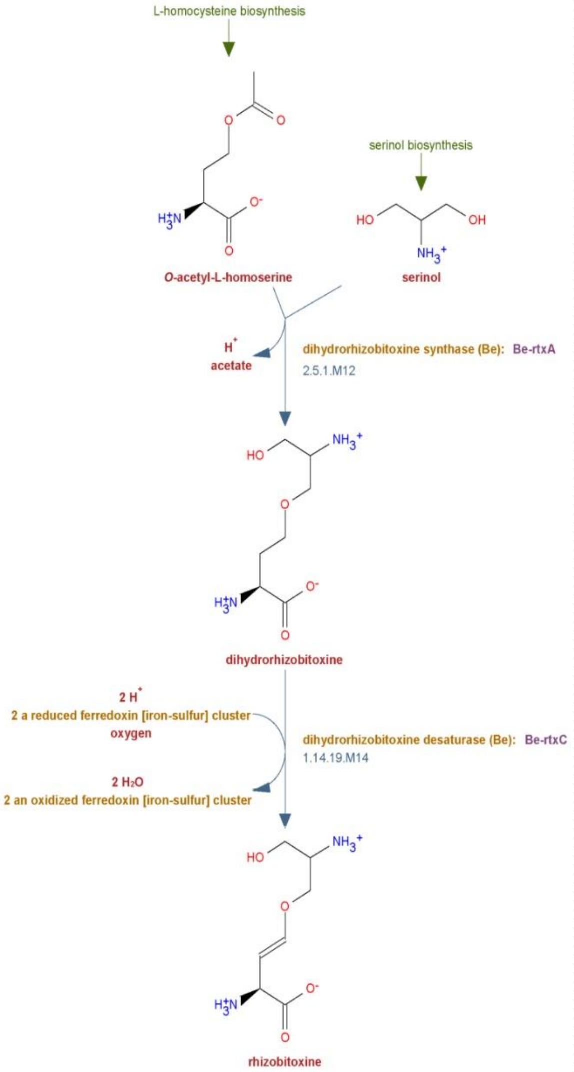
| | |
|---|---|
| Chemical Formula | $C_{13}H_{18}O_7$ |
| Molecular Weight | 286.28 Daltons |
| Monoisotopic Mass | 286.1052529325 Daltons |

Reactions in which this compound participates as a substrate

| Reactions known to consume this compound |
|---|
| a β-D glucoside + $H_2O$ → a non glucosylated D-glucose acceptor + D-glucopyranose |

| Reactions known to produce this compound | Pathways |
|---|---|
| UDP-α-D-glucose + salicyl alcohol → salicin + UDP + $H^+$ | salicin biosynthesis |
| helicin + a reduced electron acceptor → salicin + an oxidized electron acceptor | |
| a β-D-fructofuranoside + $H_2O$ → β-D-fructofuranose + a glycoside | |

| Transport Reactions |
|---|
| $\text{salicin}_{[\text{extracellular space}]} + H^+_{[\text{extracellular space}]} \rightarrow \text{salicin}_{[\text{cytosol}]} + H^+_{[\text{cytosol}]}$ |
| an [HPr protein]-$N^{\pi}$-phospho-L-histidine + $\text{salicin}_{[\text{periplasm}]} \rightarrow \text{salicin 6-phosphate}_{[\text{cytosol}]}$ + an [HPr]-L-histidine |



# ROLE OF META CYC

- ❑Used as an aid in teaching biochemistry and is a resource for metabolic engineering.
- ❑ The modification of a metabolic network through Genetic engineering involves
    - ➢Inserting a new enzyme or pathway into an organism
    - ➢Replacing an existing enzyme or pathway into an organism
    - ➢Removing an enzyme or pathway

# REFERENCES:

Kanehisa,M.and Got o ; KEGG:Kyoto Encyclopedia of Genes and Genomes. Nucleic acids Res.

https: //www.genome.jp/kegg/kegg a.html

https://www.ncbi.nlm.nih.gov/pmc/articles/ PMC102409/

# THANK YOU!!