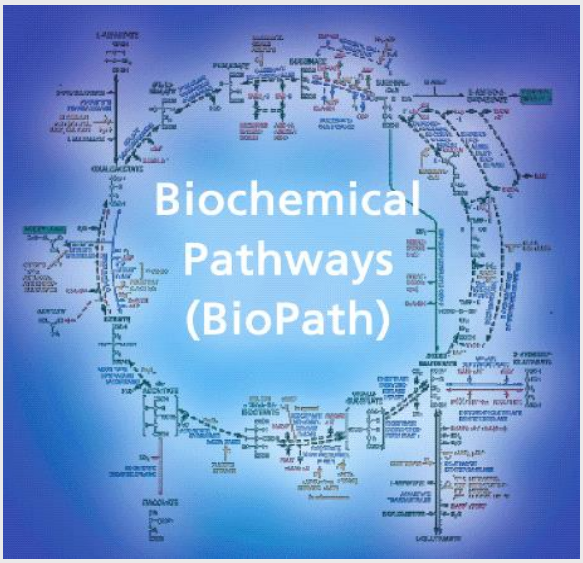
BioPath

Biochemical Pathways Database

BioPath is a database of biochemical pathways that provides access to metabolic transformations and cellular regulations derived from the "Biochemical Pathways" wall chart and additional literature harvesting. With its emphasis on chemical structure and reaction information **BioPath** offers a variety of novel applications for drug target identification and the modeling of biological systems.



All structure and reaction information in **BioPath** is stored on an atomic level allowing for direct access to all atoms and bonds of all metabolites and to the bonds broken and made during an enzymatic reaction.

Areas of Application

- Planning of metabolic engineering experiments
- Gaining deeper insights into the mechanism of enzymatic transformations
- Analyzing isotope labeling experiments
- Searching for novel enzyme inhibitors

Key Features

- Molecules with connection tables including stereochemical information
- Biochemical reactions stoichiometrically balanced, with marked reaction centers and atom-atom mapping numbers between substrates and products
- Information on enzymes (name and EC) and pathways (names)
- List of synonyms for molecule names
- Covered organism: prokaryotes, plants and yeasts, animals and general pathways
- All information manually quality-controlled

Versions

- **BioPath** database in MOL/RDFile format (optionally SQLite database) for integration into in-house database and retrieval systems
- **BioPath.Explore** (see overleaf), **BioPath** database integrated into an easy-to-use, web-based retrieval system developed and hosted by Molecular Networks

Reference

- Reitz, Sacher, Tarkhov, Trümbach, Gasteiger *Org. Biomol. Chem.* **2004**, *2*, 3226-3237. DOI: 10.1039/B410949J

MN AM

mn-am.com

BioPath.Explore

Biochemical Pathways Database & Retrieval System

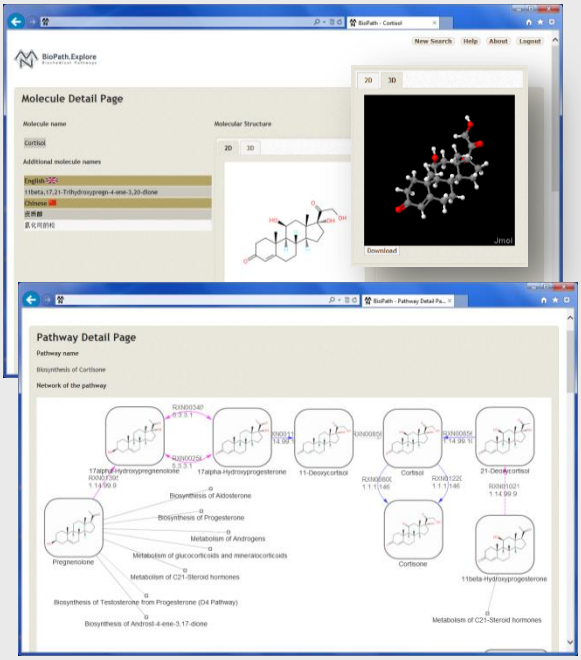
BioPath (see overleaf) is available in combination with an easy-to-use, web-based data warehouse and retrieval system developed by MN-AM.

BioPath.Explore provides a convenient electronic access to the entire information stored in the **BioPath** database by a variety of text, structure, reaction and pathway search and retrieval techniques.

All information about the metabolic molecules, reactions and enzymes are fully cross-linked which facilitates a deep and broad exploration and a state-of-the art visualization of the biochemical pathways.

Additional information, such as computed physicochemical properties and 3D molecular models, allows for a wide range of applications of **BioPath**.

Due to its web-based client/server architecture, **BioPath.Explore** can be easily integrated into an existing IT environment.



Key Features

- Enzyme name and EC number searches
- Structure search methods
- Pathway searches including shortest pathway between two molecules
- Property and text searches
- Search for shortest paths between two molecules/substrates
- Interactive pathway visualization
- 3D molecular models generated by CORINA Classic for 3D structure visualization
- Computed physicochemical properties such as molecular weight or log*P*
- Optional links to 3rd party databases

System Requirements

- **BioPath.Explore** server hosted on web server of MN-AM (for commercial version login account is required)
- **BioPath.Explore** client is platform-independent and runs with Microsoft Internet Explorer or Mozilla Firefox

Test Version

BioPath and **BioPath.Explore** can be tested free of charge online at the web site of MN-AM at mn-am.com/biopath3/.

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