



ChemEffect® Understanding the Biological Effect of Compounds

Connecting the actions of drugs and toxins on cell processes, pathways and disease.

Pathway Studio® Fact Sheet

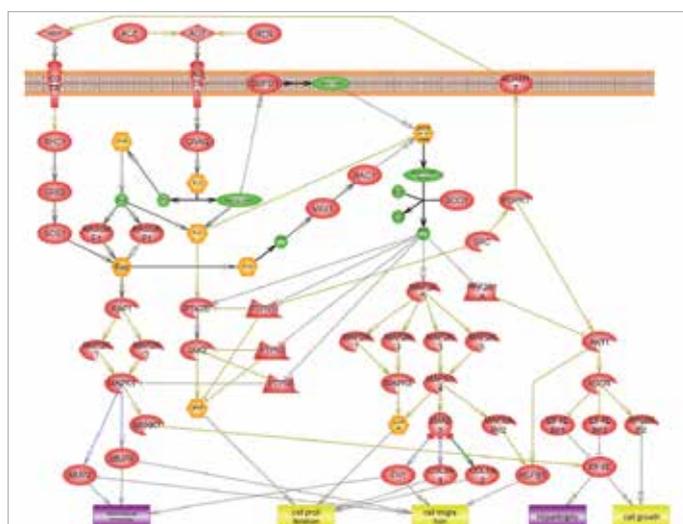
Pharmaceutical research and development requires detailed knowledge of how compounds affect biological systems in order to advance drug candidates, help confirm findings, explain mechanisms of drug action or toxicity, and identify alternative indications for drugs. Elsevier's ChemEffect® database for Pathway Studio links published information on small molecules, chemicals, and approved drugs to their effects on proteins, pathways, and cellular processes, enabling scientists to quickly:

- Identify compounds affecting target pathway(s) or proteins
- Identify targets affected by compounds similar to one(s) under investigation
- Survey known side-effects associated with compounds, and
- Use in-house experimental data to build hypothetical associations between a compound and potential phenotypical outcomes (efficacy, side effects, and drug-drug interactions)

APPLICATIONS OF CHEMEFFECT INCLUDE:

- Developing hypotheses for mechanism of toxicity or drug action
- Identifying potential alternative drug indications
- Deducing drug-drug interactions
- Correlating drug action with potential side effects

Using ChemEffect in combination with Pathway Studio, researchers can extrapolate the effects of studied drugs to make inferences about novel compounds under investigation.



ChemEffect includes innovative technology that allows researchers to scan published literature and proprietary information, extract biological relationships and integrate findings. Researchers can use their own experimental data, reference or proprietary pathways, and Pathway Studio's advanced algorithms to validate in silico hypotheses. With Pathway Studio®, ChemEffect serves as a powerful investigative tool and a one-of-a-kind knowledge hub housing integrated biological facts that advance discovery through interactive, interpretative networks.

Figure 1. ROS in angiotensin-mediated cardiovascular remodeling and hypertrophy

Angiotensin II, the active form of the angiotensinogen (AGT) precursor, is one of the most important vasoactive agents involved in the development of hypertension, cardiovascular remodeling, and hypertrophy

INCLUDED IN THE CHEMEFFECT DATABASE

- Protein–small molecule binding interactions
- Direct effects of drugs on protein targets
- Effects of drugs on gene expression and protein activity
- Observational effects of drugs on downstream proteins
- Reactions involving drugs with specific enzymes and products
- Biological effects of drugs and small molecules on cell processes and diseases

FUNCTIONAL FEATURES

- Analyze and interpret gene expression, proteomics, and metabolomics data
- Analysis of time–dose studies, toxicology mechanistic analysis, siRNA studies, microRNA data
- Gene Set Enrichment Analysis (GSEA) and Sub-Network Enrichment Analysis
- Various visualization and network building algorithms

CONFIGURATION

ChemEffect is available as an additional component to Pathway Studio and compliments the Pathway Studio Mammalian Database and DiseaseFx® Database. ChemEffect includes:

ChemEffect Database: More than 994,000 unique biological facts and relationships linked to thousands of molecules (approved drugs, small molecules, and chemicals), and supported by thousands of research and millions of literature references.

Elsevier Text Mining Technology: Patent-pending extraction technology to enrich your ChemEffect Database with additional facts from internal reports, documents, and subscriptions.

EXPERIMENTAL DATA SUPPORTED

- Gene expression
- Proteomic data
- Metabolomic data
- And others (please inquire)

GET PATHWAY STUDIO NOW

Elsevier offers customers access to Pathway Studio through flexible subscription programs. We will tailor subscription programs to fit customer needs based on the scale and configuration of the Pathway Studio deployment.

Enterprise Edition

The Enterprise Edition software provides powerful visualization and data mining tools for open-ended questioning so users can explore canonical pathways and build de novo network based on queries. They can import experimental data to develop or verify a mechanistic hypothesis, or perform limited text mining using the embedded NLP text mining Technology to customize their database content, and to capture domain specific knowledge. Multiple independent researchers in one facility can share data in the Enterprise Edition using the export and import tools. With the Enterprise Edition software, standalone access or shared access is possible.

Web Edition

The Pathway Studio Web Edition software provides web-based access to researchers almost anywhere. Elsevier provides a comprehensive knowledgebase to cover most common research areas in pharmaceutical companies, biotech, and academic research. These databases include relationships derived by Elsevier from public and private data sources, including data retrieved using the NLP text mining technology, and manually curated pathway data. Updates are available on a weekly basis.

Pathway Studio comes with either the Mammalian Database or the Plant Database, depending on your research interests.

Subscribers can add “premium data sets” to their subscription, including:

- DiseaseFx, a disease-centric database for the study of the molecular cause and effects of disease on cellular processes

Web databases are updated weekly, while the Enterprise database is updated quarterly.



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For more information on how this versatile, scalable solution can help you and your team, visit:

elsevier.com/products/solutions/pathway-studio