

# VitaPad

A graphical editing tool for  
pathway diagrams.

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# Pathways

- Networks of relationships between biological entities
- Scope ranges from sub-cellular to across multiple organs
- Knowledge of pathways facilitates interpretation of experimental data

# The Problem

- Pathway definitions are highly subjective and constantly exposed to new information
- Pathway software is limited if it cannot be readily extended to new classes of pathway-related data

# The Solution

Software for pathway visualization must employ a flexible and extensible design:

- Driven by 'metadata'
- Loose coupling between biological data and graphical information

# Other Objectives

- Open-source, including open standards for XML and database storage
- High-resolution graphics, with responsive user interface and fully customizable graph appearance
- Sophisticated automatic graph layout

# Program Functions

- I. Create original pathway diagrams
- II. Edit existing diagrams
- III. Add experiment data to diagram
- IV. Use layout algorithms to automatically generate diagrams
- V. Store diagram as XML file
- VI. Persistence of diagrams in a database



# Basic Graph Structure

Graph structure is independent of scientific context.

Format is typical of network graphs:

- Nodes (Vertices) - e.g. Chemical compounds
- Edges - e.g. Chemical Reactions
- Decorations - e.g. Catalysts, Expression values



# Rendering

Rendering process is independent of domain-specific knowledge.

- Concerned with abstract 2D shapes, not biological concepts like genes, compounds
- New data classes can be rendered simply by detailing their appearance in the database
- Three levels of graphics customization: global level, pathway level and object level

# Layout Algorithm

VitaPad uses a “spring-embedded” algorithm to automatically lay out pathways:

- It uses a virtual physical model to establish the ideal location for elements on the graph.
- It is particularly effective for complex, partially-cyclical graphs such as metabolic pathways.

# Mapping Experiment Data

- Microarray data is gathered from the database
- Data values are mapped onto the pathway graph next to their corresponding gene
- Visual appearance can be modified through a customizable gradient

VitaPad

File Edit Mode

**Edit Panel**

Define the gradient to use

6,017.642  
4,534.656  
3,051.671  
1,568.685  
85.7

Colors

Min:

Max:

Mid: N/A

No Value:

Values

Min:

Max:

Save Type Load OK Cancel

**Display Panel**

Pathway:  
Alanine and aspartate metabolism

Species:  
Hs

Experiment:

Annotate Go To KEGG

# Database Persistence

VitaPad is backed by the iSpar database, which provides information on pathway elements and experimental data.

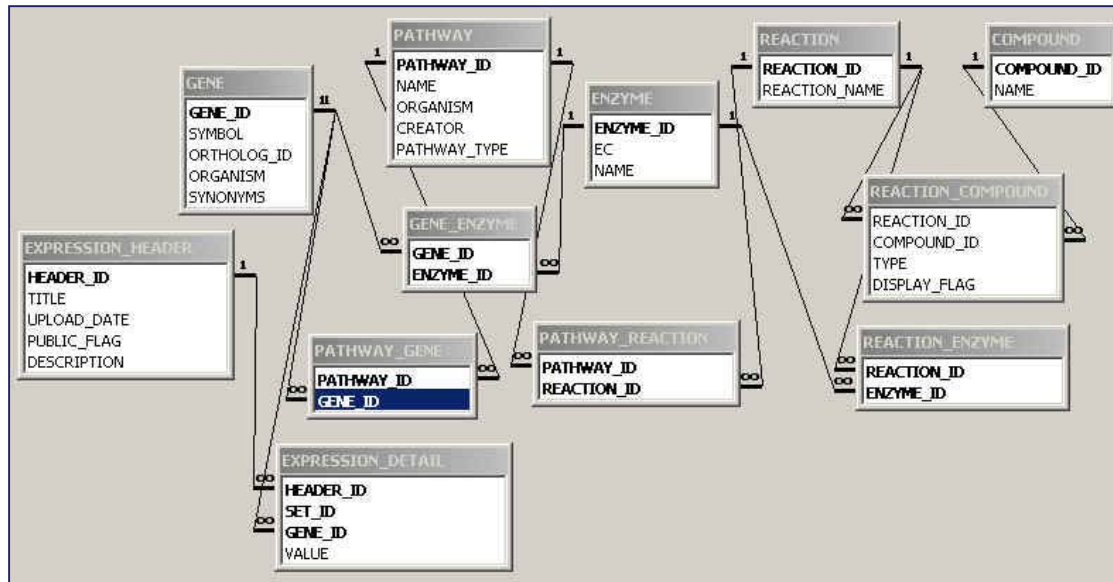
In addition, we provide a schema to allow the end user to build their own database for pathway storage.

# Database Features

- Biological details are separated from rendering details
- This allows new classes of data, unknown to the original database, to be added easily
- Makes the program more flexible and extensible

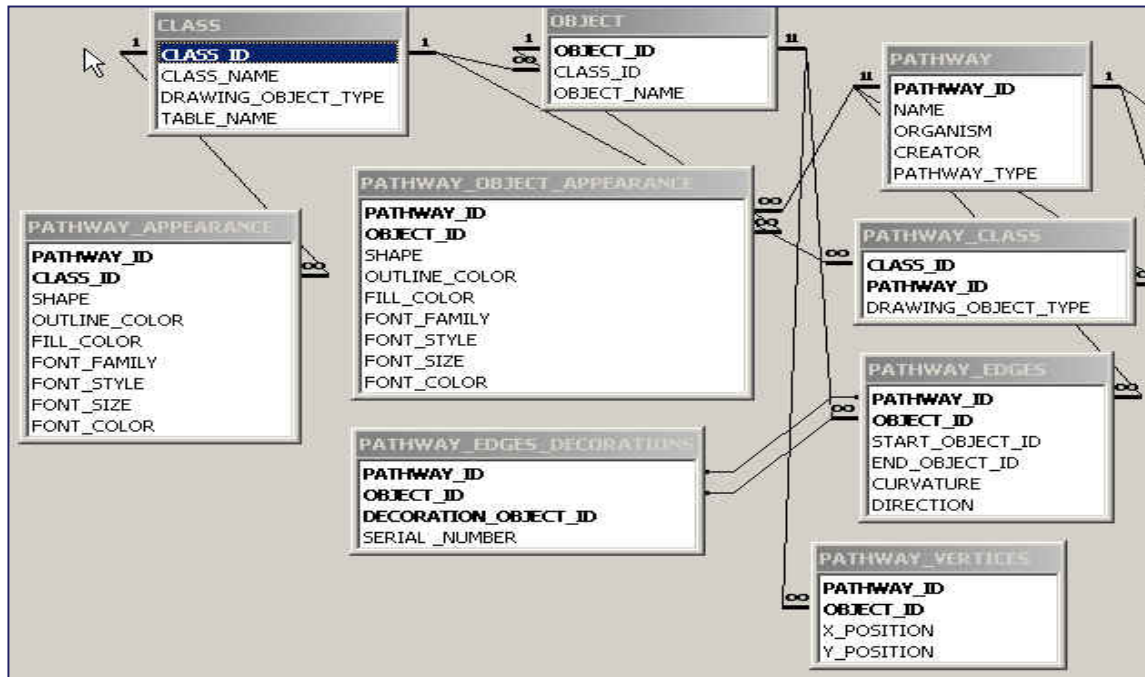
# Database Structure

## Biological Details



# Database Structure

## Rendering Details





# XML Persistence

VitaPad uses XML to store and transport individual pathway files. An XML format offers several advantages:

- Widely-used, many parsers available.
- Plain-text format, easy-to-read.
- Standardized across multiple platforms.

# VitaPad XML Example

```
<VERTEX id="28736">
  <vertDataClass annotation="" id="C02984"
    name="L-Aspartyl-tRNA(Asp)"/>
  <xposition>1162</xposition>
  <yposition>410</yposition>
  <vertShape>Rectangle</vertShape>
  <vertOutlineColor>-
    16777063</vertOutlineColor>
  <vertFillColor>-3355393</vertFillColor>
  <vertFont>Palatino Linotype_0</vertFont>
  <vertFontSize>10</vertFontSize>
  <vertFontColor>-16777216</vertFontColor>
  <on-link>-1</on-link>
  <on-link-position>-1.0</on-link-position>
</VERTEX>
```

```
<LINK id="28652">
  <vertexA>28648</vertexA>
  <vertexB>28650</vertexB>
  <direction>Forward</direction>
  <curvature>0.0</curvature>
  <linkColor>-8388608</linkColor>
  <solid>Y</solid>
  <DECORATION className="Enzyme"
    id="28653">
    <decDataClass altName="2.6.1.2"
      annotation="" id="EN1714"
      name="Alanine transaminase"/>
    <decShape>Ellipse</decShape>
    <decOutlineColor>-
      16764160</decOutlineColor>
    <decFillColor>-10040769</decFillColor>
    <decFont>Trebuchet MS_0</decFont>
    <decFontSize>9</decFontSize>
    <decFontColor>-6750208</decFontColor>
  </DECORATION>
</LINK>
```