# BioPath\*

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### **1** Short Description

Biochemical processes in organisms are considered as very large networks consisting of reactants, products and enzymes with interconnections representing reactions and regulation. Examples are given by the well known *Boehringer poster* [4] and the *Biochemical Pathways* atlas [5]. These networks are very complex and grow fast by the steady progress of knowledge in life sciences.

BioPath is the result of the Electronic Biochemical Pathways Project [1,3], a joint work of research groups at the universities of Erlangen, Mannheim, Passau and Spektrum Verlag, Heidelberg. BioPath provides a convenient electronic access to biochemical reactions at a high level of detail and explores all advantages of an electronic version over a printed one. It uses an innovative algorithm for drawing directed graphs [7] based on Graphlet [2].

# 2 Layout Algorithm and Layout Features

The state of the art in the visualization of biochemical reaction networks are manually produced drawings, as they appear in textbooks, on the poster [4] or in electronic information systems. *BioPath* is the first tool with a dynamic visualization of pathways, which meet the following requirements:



Fig. 1. Example

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**Local.** Components of the reactions should be placed in the established drawing style of biochemistry as in textbooks.

Global. All reactions should be placed according to their temporal order.

**Context sensitive navigation and views.** The drawing should maintain the mental map when the granularity of the provided information changes by a new view [6].

As biochemical pathways can be represented by graphs, the visualization of the objects and their connections is a typical graph drawing problem. However, common algorithms are insufficient to represent pathways according to the established conventions of biology and chemistry. Our new customized algorithm produces hierarchical layouts of directed graphs taking node sizes and constraints into account. The sizes of the nodes enforce a new layering strategy. This leads to compact drawings. Using constraints we can draw distinguished paths differently, e.g. the citrate cycle as a real cycle, and we preserve the mental map of the user in sequences of related drawings. The algorithm is described in [7].

## 3 Architecture

BioPath is a classical 3-tier web application based on *Graphlet* and the Java<sup>TM</sup> Servlet Technology. See Figure 2 for an architecture overview.

The web interface and query engine are written in Java. They access Graphlet and the database interface which are written in C++ via the Java Native Interface (JNI).

#### 4 Screenshot

Figure 1 shows a layout generated by *BioPath*. See also [1].



Fig. 2. BioPath Architecture

#### References

- 1. Biopath: Biochemical pathways. http://biopath.fmi.uni-passau.de, 2000.
- 2. M. Himsolt. Graphlet: Design and implementation of a graph editor. Software -Practice and Experience, 30(11):1303–1324, 2000.
- C.-C. Kanne, F. Schreiber, and D. Trümbach. Electronic Biochemical Pathways. In *Proc. 7th Symp. on Graph Drawing (GD'99)*, volume 1731 of *LNCS*, pages 418–419. Springer Verlag, 1999.
- 4. G. Michal. Biochemical Pathways (Poster). Boehringer Mannh., Penzberg, 1993.
- 5. G. Michal. Biochemical Pathways. Spektrum Akad. Verlag, Heidelberg, 1999.
- K. Misue, P. Eades, W. Lai, and K. Sugiyama. Layout adjustment and the mental map. J. of Visual Languages and Computing, 6:183-210, 1995.
- 7. F. Schreiber. Visualisierung biochemischer Reaktionsnetze. PhD thesis, Universität Passau, 2001.