K-VIZ: KEGG BASED VISUALIZATION FOR COMPARING METABOLIC PATHWAYS

Dong-Hyuk Im

Department of Computer Science and Engineering, Seoul National University
San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-742, South Korea
dhim@idb.snu.ac.kr

Dong-Hee Lee

Department of Computer Science and Engineering, Seoul National University
San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-742, South Korea
leedh@idb.snu.ac.kr

Hyoung-Joo Kim

Department of Computer Science and Engineering, Seoul National University
San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-742, South Korea
hjk@snu.ac.kr

ABSTRACT

The comparison of metabolic pathway in different species is important in detecting a missing gene. There are many visualization tools for metabolic pathway. However, biologists need not only visualization of one pathway but also visualization for comparison among pathways. K-Viz is a tool for visualization of metabolic pathway based on KEGG. To compare among pathways in different species, K-Viz uses different colors on each species for path expression such as PathComp in KEGG and shows the table of path in pathway. K-Viz helps biologists to understand the comparison among metabolic pathways in different species.

KEYWORDS

Visualization, KEGG, Metabolic pathway

1. INTRODUCTION

Pathway represents the networks of chemical reactions from a compound to another compound by an enzyme. It is important to compare among pathways in different species in order to understand the function of proteins. There are a variety of existing pathway systems. These tools (Alexander, 2002) only focus on the visualization of one pathway and detection of incomplete pathways in one species. A general approach to compare among pathways is to draw a pathway and to use different colors for each species. The drawback of this method is that comparing pathways in many species is very difficult due to the limited number of colors.

In this paper, our approach extends coloring method by taking into consideration the frequency of enzymes. The basic idea is that we count enzymes that appear in the same path in different species and apply color corresponding to the number of times. To address the problem of the missing gene, we show additional table of enzymes. This table helps to detect the missing gene in a pathway. It is possible to compare pathways easily by our visualization tool.

2. K-VIZ

The goal of K-Viz is to achieve a visual comparison of metabolic pathways. K-Viz is a visualization based on KEGG (Kanehisa, 2000). K-Viz is web-based and implemented in java. We extract all metabolic pathway

maps and data from KEGG(e.g. KGML). We transform these data to RDF using XSLT and use Sesame (J. Broekstra, 2002) as a storage. The comparison of pathways in K-Viz can be summarized as follows: 1) as input, the initial compound, the final compound and species are selected. 2) We compute each path expression from the initial to the final in selected species. 3) We then create only one enzyme list by overlapping all path expressions. 4) We finally assign the color matching the frequency count to enzyme node in a pathway map. Figure 1 shows an example of comparison in K-Viz.
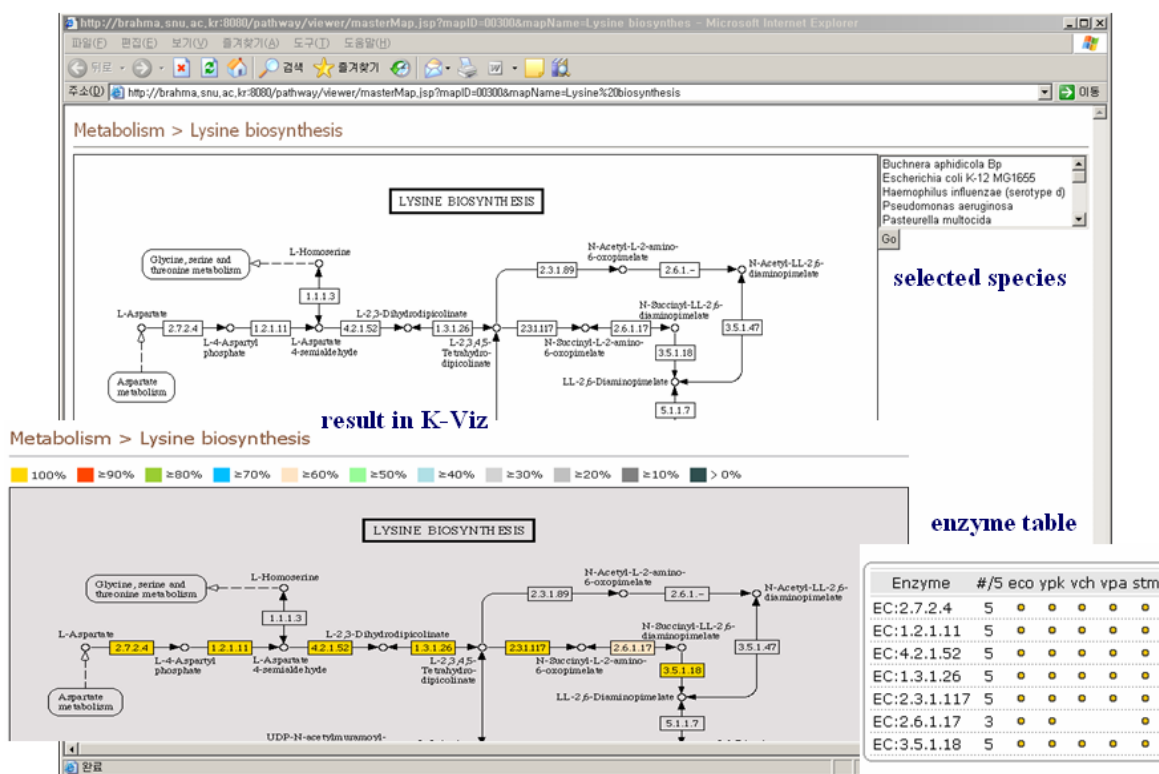

Figure 1. A visual comparison of pathways

It allows the user to compare the part of interest in pathway. The results, in Figure 1, show that we can find the missing gene in EC:2.6.1.17 position. In the future, our visualization for comparison can be used to analyze a missing gene.

ACKNOWLEDGEMENT

REFERENCES

Alexander Goesmann et al, 2002. PathFinder: reconstruction and dynamic visualization of metabolic pathways. *BIOINFORMATICS*, Vol. 18, No. 1 ,pp 124-129

Kanehisa, M. et al, 2000. KEGG: kyoto Encyclopedia of Genes and Genomes. *Nucleic Acid Research*, Vol. 28, No. 1 ,pp 27-30

J. Broekstra et al, 2002. Sesame: An Architecture for Storing and Querying RDF Data and Schema Information. *International Semantic Web Conference*, Sardinia, Italy.