

Web-based Zoomable Pathway Browser using KEGG Atlas and Google Maps API

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Abstract

Biological pathways provide a systematic context in the interpretation of the huge masses of “omics” data. Traditional pathway maps available in public web databases used to be static and subdivided into individual pathways, but recent web technologies allows the interactive use of global maps via zoomable user interface (ZUI) and AJAX (Asynchronous XML and Javascript) web development paradigm. Here we introduce a web-based zoomable pathway browser using the global metabolic pathway map of KEGG Atlas and Google Maps API for ZUI. This web application allows numerous interactive queries and data mining, as well as data mapping from metabolome, proteome, and transcriptome experimentas.

Keywords: metabolic pathway, visualization, KEGG Atlas, Google Maps API

1 Introduction

With the increasing focus on systems biology approaches, interpretation of high-throughput “omics” data is often required to be studied in the context of biological pathways. Although most existing pathway databases used to be static and subdivided into specific pathways primarily due to the limitations of web development technologies, recent introduction of AJAX (Asynchronous XML and Javascript) paradigm and success of Google Maps for the representation of geographical information inspired the exploratory use of interactive zoomable user interface (ZUI) for genomics and systems biology [1]. However, existing websites are often limited in their interactivity for complex data queries, ZUI, and mapping abilities of high-throughput experimental data. Here we introduce a novel web application that provides interactive ZUI-based access to pathway information rebuilt from the global map of KEGG Atlas [2]. Key features of this web application includes data mapping for metabolome, proteome, transcriptome data, path search between two compounds, database query and access to information in UniProt KB and KEGG, metabolic reconstruction from amino acid sequences, and collaborative manual editing of map diagrams and annotations.

2 Method and Results

2.1 User Interface.

ZUI is developed using the popular Google Maps API [3], and AJAX software interface is created with Ext JS 2.0 framework [4]. Therefore, the software interface supports interactive queries and smooth zooming with mouse scroll wheels. Users can easily annotate and edit the maps by placing custom markers, drawing

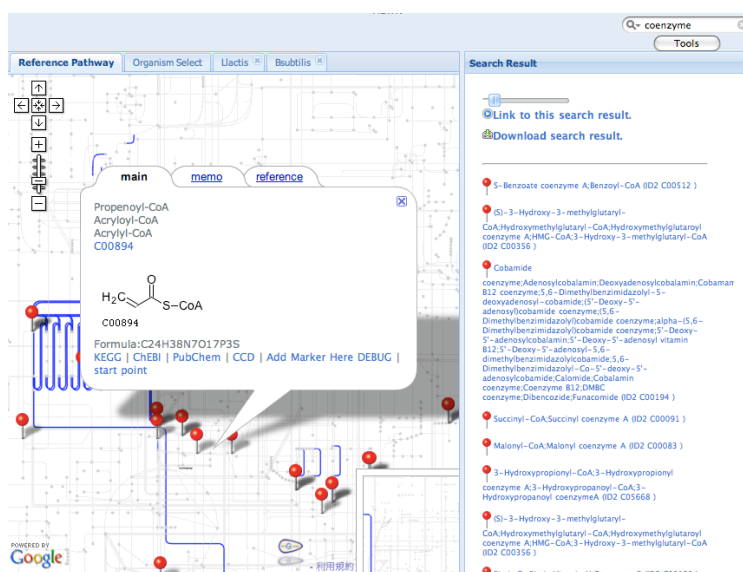
lines, and by adding custom comments and annotations that can be shared among researchers.

2.2 Search

This system has database backend based on KEGG and UniProt. Search system supports many query type such as keyword, atomic mass number with range for compounds, and path search between two compounds. Detailed information about the components can be quickly invoked by clicking on the edges and nodes of the pathway map, that contain hyperlinks for further searching.

2.3 Data Mapping

Users can map their own data onto the map, by changing the size, color, shapes or icons, and the arrowhead of edges. Edges and nodes can be specified with KEGG IDs, gene names, and EC numbers.



The screenshot displays a web application interface for a metabolic pathway map. The main window shows a network of nodes and edges representing a pathway. A search bar at the top right contains the text "coenzyme". Below the search bar, there are options to "Link to this search result" and "Download search result". The search results are listed on the right side of the interface, including:

- 5-Benzoate coenzyme A: Benzoyl-CoA (ID2 C00512)
- (S)-3-Hydroxy-3-methylglutaryl-CoA, Hydroxymethylglutaryl coenzyme A: HMG-CoA, 3-Hydroxy-3-methylglutaryl-CoA (ID2 C00356)
- Cobamide
coenzyme: Adenosylcobalamin, Deoxyadenosylcobalamin, Cobamarn B12 coenzyme: 5,6-Dimethylbenzimidazolyl-5'-deoxyadenosylcobamide (S'-Deoxy-5'-adenosylcobamide coenzyme: (S,6-Dimethylbenzimidazolylcobamide coenzyme: alpha-(S,6-Dimethylbenzimidazolylcobamide coenzyme: (S'-Deoxy-5'-adenosylcobalamin, (S'-Deoxy-5'-adenosyl vitamin B12, (S'-Deoxy-5'-adenosyl-5,6-dimethylbenzimidazolylcobamide, 5,6-Dimethylbenzimidazolyl-Co-S'-deoxy-5'-adenosylcobamide, Calamide, Cobalamin coenzyme: Coenzyme B12, DMBC coenzyme: Dibencoside, Funsoside (ID2 C00194)
- Succinyl-CoA, Succinyl coenzyme A (ID2 C00091)
- Malonyl-CoA, Malonyl coenzyme A (ID2 C00083)
- 3-Hydroxypropionyl-CoA, 3-Hydroxypropionyl coenzyme A, 3-Hydroxypropanoyl-CoA, 3-Hydroxypropanoyl coenzyme A (ID2 C03568)
- (S)-3-Hydroxy-3-methylglutaryl-CoA, Hydroxymethylglutaryl coenzyme A: HMG-CoA, 3-Hydroxy-3-methylglutaryl-CoA (ID2 C00356)
- Biotin, Biotin, Vitamin H Coenzyme, B (ID2 C00120)

The main window also shows a detailed view of a node, "Propenyl-CoA", with its chemical structure and associated information:

Propenyl-CoA
Acryloyl-CoA
Acrylyl-CoA
C00894

C=CC(=O)S[CoA]

Formula: C24H38N7O17P3S
KEGG | ChEBI | PubChem | CCD | Add Marker Here | DEBUG | start point

Figure 1: Screenshot of the web application

3 Discussions

This application provides an intuitive interface as a gateway to many online resources related to systems biology. Highly interactive user interface with ZUI and AJAX is especially suitable for the browsing of large pathway maps, and the ability to edit, annotate, share, and map custom information will assist omics researchers.

References

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