

Community-based Linking of Biological Network Resources: Databases, Formats and Tools

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Summary

The analysis of biological networks is increasingly important in the life sciences and in particular in systems biology. Computer-based analysis tools are exploited for the investigation of these networks. However, to find relevant data sources can be a time-consuming task, access to information changes, frequently it is not obvious to a user which tools can be used in combination with specific data sources, and network data is often not available in a format directly usable by analysis tools.

To assist in collecting information about biological network data sources, and to help in investigating possible combinations of data sources and analysis software, we created BiNCo-wiki. BiNCo-wiki is a wiki system that stores information related to biological networks and allows all users to add or modify this information in an easy way. The collaborative character of a wiki system supports easy sharing of information and allows the community-based extension of the information already stored in BiNCo-wiki. We describe the general structure and functionality of the system and its initial content. BiNCo-wiki is accessible, free of charge, at <http://pgrc.ipk-gatersleben.de/BiNCo-wiki>.

1 Introduction

Biological networks are abstract representations of biological systems and their analysis is a growing field in modern biology. As the networks are often very large, software tools are used for their investigation. Examples are tools to find network motifs or to rank network elements according to centrality measures. However, there is a problem with the availability of network data in a format that is readable for analysis software. On one hand there are various databases that store and export information in different file formats. On the other hand there are various computer programs that are restricted to specific file formats and do not have the ability to read all of those formats. Researchers either have to use a large number of different analysis software or are bound to use the information stored in only some of the available data sources. Nevertheless, some software can be used to open specific file formats and save the data in different file formats. Therefore it would be very useful to have information about all different ways to exchange data between data sources (e. g. databases) and analysis tools.

To overcome this problem and to assist users in finding possible combinations of data sources and analysis software, we created BiNCo-wiki (BIological Networks and CONverter wiki). BiNCo-wiki is a wiki system that stores information related to biological networks – databases, file formats, software, and literature – and allows users to add or modify this information.

BiNCo-wiki

Welcome

Welcome on the BiNCo-wiki website!
 BiNCo-wiki is a project that wants to offer a platform to present a collection of information on data sources for biological networks, file formats that save biological networks and software to analyze the information of these sources.
 All entries of BiNCo-wiki can be connected. These links can be used to identify dependencies.

The last 5 entries

View	Type	Name	Shortname	URI	Last Change	License Type
View	Software	GML to PajekNet	Gml2PajekNet	-	2007-07-26	Free access / Freeware
View	Publication	Expression dynamics of a cellular metabolic network	Expression dynamics of a cellular metabolic network	web site	2007-06-13	Free access / Freeware
View	Publication	Transcriptional Regulatory Networks in <i>Saccharomyces cerevisiae</i>	Transcriptional Regulatory Networks in <i>Saccharomyces cerevisiae</i>	web site	2007-06-13	Free access / Freeware
View	Publication	Reconstruction of metabolic networks from genome data and analysis of their global structure for various organisms	Reconstruction of metabolic networks from genome data and analysis of their global structure for various organisms	-	2007-06-13	Unknown
View	Database / Data file	BioWarehouse	BioWarehouse	web site	2007-06-12	Open access / Open source

Information on BiNCo-wiki

Number Of Entries	54
Number Of Connections	62
Number Of Users	6

Navigation

- Feedback
- View List of all entries
- Search Entries
- Login
- Register
- Help

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Figure 1: Screen shot of the BiNCo-wiki home page. On this page a welcome message, the five newest entries, and statistical information are displayed. The tab bar (top right) is visible on every page.

The collaborative character of a wiki system supports easy sharing of information and allows the extension of the information already stored in BiNCo-wiki. BiNCo-wiki is located at <http://pgrc.ipk-gatersleben.de/BiNCO-wiki>, see Fig. 1 for a screen shot.

This paper is structured as follows. Section 2 gives a short introduction into wiki systems, presents the general structure of BiNCo-wiki and briefly deals with implementation aspects of the system. Section 3 gives an overview of the functionality of the system. Two application examples of BiNCo-wiki are presented in Sect. 4. In Sect. 5 the system is compared to similar databases of pathways and networks. The initial content of the system is summarized in the conclusion in Sect. 6.

2 BiNCo-wiki

2.1 Collaborative software and Wiki systems

Wiki systems [5, 14, 19] are collaborative software systems which provide a set of web pages that are accessible and changeable worldwide. The first available wiki system was the WikiWikiWeb started in 1995 by Ward Cunningham on the web site <http://c2.com/cgi/wiki/> [5]. A well known wiki system is the free encyclopedia Wikipedia [19]. The intention of creating wiki systems is to help users to make information available in a fast, uncomplicated, and collaborative manner. Therefore the web pages can be edited, links to other pages can easily be created, and new pages can be added simply by using a web browser. Modern wiki systems store different revisions of pages and therefore give access to previous versions of each page.

BiNCo-wiki is a wiki system designed to collect and present information on databases, data

files, publications, file formats, and software concerning biological networks. The intention of this collection is to help researchers to find requested information faster. As related entries in BiNCo-wiki are connected by links, visitors can even find information which would be difficult to obtain in other ways. Links in BiNCo-wiki allow a user, for example, to find export formats of databases and related file formats used in analysis software. This may help in finding the appropriate analyzing software to investigate a specific biological network.

2.2 Users and objects

BiNCo-wiki users are divided into three groups: visitors, users, and administrators. A **visitor** is a person browsing the BiNCo-wiki web site. A visitor is not logged in to the system. A person that is logged in using a user name is called a **user**. A user has the additional privileges of an **owner** over the entries they personally created. Owners are allowed to edit the corresponding entry. **Administrators** are allowed to modify all entries and the user information of every user. The three groups are structured hierarchically, an administrator is also a regular user and a user is also a visitor.

The information stored in BiNCo-wiki is divided into four **object classes**: database / data file, publication, file format, and software. Each single instance of the four classes is called an **object** in BiNCo-wiki. **Entries** in BiNCo-wiki represent the information contained in one object. Within each entry, the *Type* of the entry specifies the group to which the entry belongs. Every entry has a *Name* and a *Shortname* (the abbreviation or acronym of the *Name*). The *Description* documents the main features of the object and is usually extracted or summarized according to the information in the object given by the corresponding web site. The *URI* is the location of the resource. The *License* field contains the complete license text or important parts of it as well as a link to the page where the license is shown. *License Type* denotes the type of the license. Publication entries additionally have a *PubMed ID*, authors, and the year of publication. The *File format extensions* field lists all common file extensions for a given file format. *Source code snippets* are useful for other software developers. They can include these snippets in their own software. *JAR files* and *JNLP files* allow simple applications to be stored in the system and started as Java Web Start applications. The version of an entry that is displayed for all visitors is called the **active entry**. A **connection** is a record containing a relation between two entries. Connections are directed. Each connection has a source, a sink, a type, and a description.

2.3 Wiki engine and database schema

To enable the operation of a wiki system requires an underlying system that is able to save the information given by users. This system is often called a **wiki engine**. Usually the information presented by the wiki system is stored in a database. The wiki engine manages the operations on the stored information.

The database schema of BiNCo-wiki is shown in Fig. 2. To perform search operations faster, BiNCo-wiki saves the current records in one table and archives the history of records in a second table.

Oracle Application Express [20], a web application development tool for Oracle databases, was used to create the BiNCo-wiki front end. Oracle Application Express allows the creation

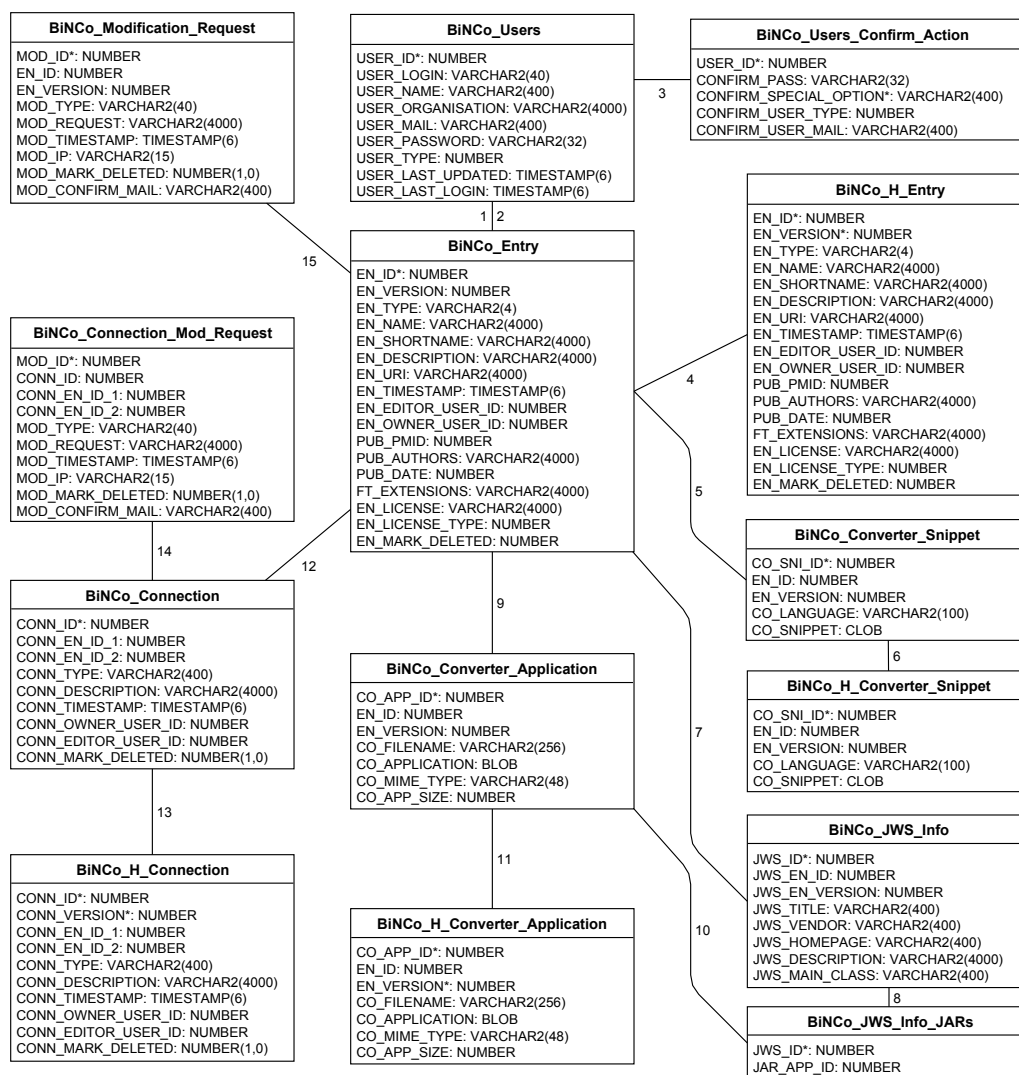


Figure 2: Database schema of BiNCo-wiki. Each box represents one table in the database. The table name is displayed in the head. Columns of each table are given below the table name. Primary keys are marked with an asterisk (*).

Foreign key relations connecting tables: 1 - BiNCo_Entry.EN_EDITOR_USER_ID → BiNCo_Users.USER_ID; 2 - BiNCo_Entry.EN_OWNER_USER_ID → BiNCo_Users.USER_ID; 3 - BiNCo_Users_Confirm_Action.USER_ID → BiNCo_Users.USER_ID; 4 - BiNCo_H_Entry.EN_ID → BiNCo_Entry.EN_ID; 5 - BiNCo_Converter_Snippet.EN_ID → BiNCo_Entry.EN_ID; 6 - BiNCo_H_Converter_Snippet.CO_SNI_ID → BiNCo_Converter_Snippet.CO_SNI_ID; 7 - BiNCo_JWS_Info.EN_ID → BiNCo_Entry.EN_ID; 8 - BiNCo_JWS_Info_JARs.JWS_ID → BiNCo_JWS_Info.JWS_ID; 9 - BiNCo_Converter_Application.EN_ID → BiNCo_Entry.EN_ID; 10 - BiNCo_Converter_Application.CO_APP_ID → BiNCo_JWS_Info_JARs.JAR_APP_ID; 11 - BiNCo_Converter_H_Application.CO_APP_ID → BiNCo_Converter_Application.CO_APP_ID; 12 - BiNCo_Connection.CONN_EN_ID_1 → BiNCo_Entry.EN_ID + BiNCo_Connection.CONN_EN_ID_2 → BiNCo_Entry.EN_ID; 13 - BiNCo_H_Connection.CONN_ID → BiNCo_Connection.CONN_ID; 14 - BiNCo_Connection.Mod_Request.CONN_ID → BiNCo_Connection.CONN_ID; 15 - BiNCo_Modification_Request.EN_ID → BiNCo_Entry.EN_ID

of dynamic pages via templates to display and edit information stored in the database. All operations not available through templates have to be implemented in PL/SQL, a procedural extension of SQL [17]. Authentication schemes are used to control access to special pages, for example the administrative pages. The decision towards Oracle Application Express was based on the IT policy of the hosting institute. To reduce maintenance efforts web applications hosted by the institute are required to use an already established environment composed of an Oracle database, Oracle Application Express and similar systems. Existing open source systems for web application or database where therefore not considered for the implementation of BiNCo-wiki.

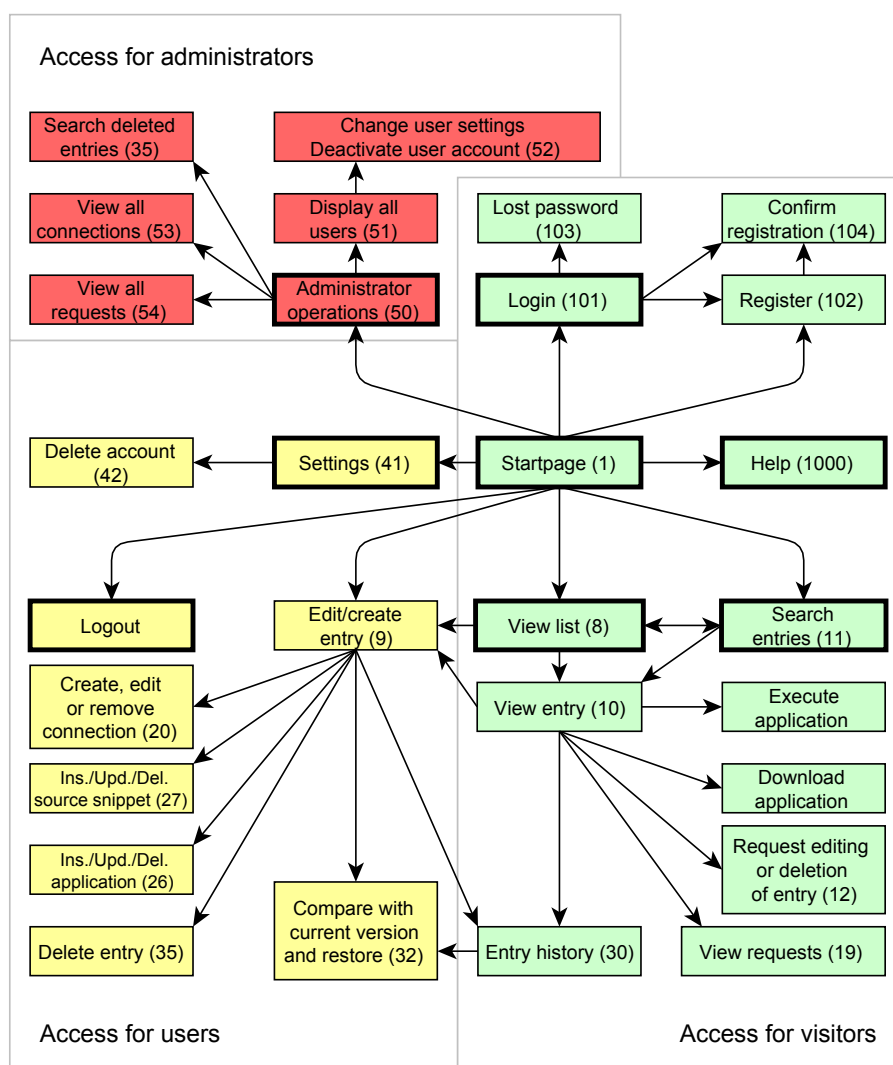


Figure 3: Site map of the BiNCo-wiki web site. Each box represents one page of BiNCo-wiki. The numbers represent the Oracle Application Express page ID. Boxes without numbers are scripts. Boxes with a bold border have a link in the tab bar. Green boxes are available for visitors, users and administrators, yellow boxes are available for users and administrators and red boxes are available for administrators only.

3 Usage of BiNCo-wiki

The web interface of BiNCo-wiki is the visible part of the system. Every action in BiNCo-wiki is performed by the users using this web interface. A screen shot of the home page is shown in Fig. 1. There are pages that are available to all visitors, pages that require authentication as a user and pages that require authentication as an administrator (see Site map in Fig. 3).

Home page and browser checks The home page (see Fig. 1) is the first page displayed when visiting BiNCo-wiki. The home page shows a welcome text, a list of the five newest entries, and information such as the number of entries and the number of connections. There are checks for *JavaScript* and cookies. If JavaScript is disabled various actions are not possible. Cookies are required by Oracle Application Express to manage the sessions of BiNCo-wiki.

Tab bar and breadcrumb list The tab bar and the breadcrumb list are visible on all pages. The tabs are direct links to the main pages whereas the breadcrumb list links to pages that are

Home > List of all BiNCo Entries > [View BiNCo Entry](#)

[Request Edition](#)

[Browse History](#)

Entry information

Entry Type: **Database / Data file**

Name: **BioModels Database**

Shortname: **BioModels**

Description: **The BioModels Database is a data resource for published, peer-reviewed, quantitative models of biological processes. The models in the database are annotated and linked to external informations like publications, pathway databases or controlled vocabularies. Currently, there are about 165 models in the database, that distinguishes between curated and non-curated models.**

URI: <http://www.ebi.ac.uk/biomodels/>

PubMed ID: 16381960

License Type: **Open access / Open source**

License information

1. The copyright on the encoded form of a model distributed by BioModels Database does not imply any copyright of the model characteristics, whether interaction graph, mathematical description or simulation results, as they are described in the original publication. Each individual model retains the copyright assigned by the author(s) of the reference publication." 2. You may distribute verbatim copies of the complete dataset or a subset of the models, provided that you duplicate this copyright notice and the disclaimers shown below. 3. You may otherwise modify your copy of any of the models in any way, provided that you also do at least ONE of the following: a. Use the modified model only within your organization. b. Contact BioModels team to include your modifications in the standard version of the model. c. Rename the modified model, and remove both the BioModels Database identifier and any mention of the model creators. See <http://www.ebi.ac.uk/biomodels/legal.html>

Connections (This entry is source)

Edit	Link	Shortname	Type	Description
Edit	Follow link	SBML	Datafile available Exports	There are two available types of downloads. 1. All Models Under SBML L2 V1 Format 2. A single SBML L2 V1 for each entry. Example: http://www.ebi.ac.uk/compneur-srv/biomodels-main/publ-model.do?mid=BIOMD0000000001
Edit	Follow link	CellML	Exports	On the page of every entry there is a link to the corresponding XML file. Example: http://www.ebi.ac.uk/compneur-srv/biomodels-main/publ-model.do?mid=BIOMD0000000001
Edit	Follow link	BioPAX Level 2	Exports	On the page of every entry there is a link to the corresponding XML file. Example: http://www.ebi.ac.uk/compneur-srv/biomodels-main/publ-model.do?mid=BIOMD0000000001

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Figure 4: View of an entry of BiNCo-wiki. This page displays all information available for an entry, here the information for the entry “BioModels”.

on the path from the home page to the current page on the site map (see Fig. 3).

List of all entries The visitor is able to view the complete list of entries on the page named “List of all BiNCo entries”. The listings can be sorted by each column. A limitation of the entry types and a simple search can be performed on this page.

Search entries To be able to perform a search with more detailed options the visitor has to go to the “Search entries” page. On this page there is a form which allows the input of search keys for all fields of the entries. The search results are displayed in the same manner as the list of all entries, see Fig. 5.

View entry The “View entry” page (see Fig. 4) contains a region which shows all information of a given entry. The URI is also displayed as a hyperlink, and the PubMed ID is displayed as a hyperlink to the corresponding PubMed page. Beneath the “Entry information” region there can be two regions that display the connections to other entries. The regions “Connections (this entry is source)” and “Connections (this entry is sink)” list the connections that start or end at the current entry, respectively. These regions display the information of the connections as well as a link to edit the connection (or to request edition if a visitor does not have sufficient rights) and a link to jump to the corresponding entry. The screen shot in Fig. 4 is an example where the “Connections (this entry is source)” region is displayed.

Register for BiNCo-wiki To register for BiNCo-wiki the visitor must enter a user name, their real name, their organization, an email address and a password on the registration page. Before

BINCo-wiki

Home > List of all BiNCo Entries > **Search Entries**

Home > List of all BiNCo Entries > **Search Entries**

Search Form

Search In All Fields

Type

☒ Database / Data file

☒ Publication

☒ File format

☒ Converter / Software

Name contains

Shortname contains

Description contains

URI contains

PubMed ID contains

Authors contains

License type

☒ Open access / Open source

☒ Free access / Freeware

☒ Free for academic use

☒ Free after registration

☒ Different License Types

☒ Purchase required

☒ Unknown

All fields are connected with a logical "and". The search is case insensitive.

View	Type	Name ▲	Shortname	URI	License Type
View	Database / Data file	aMAZE (Project discontinued)	aMAZE	URI	Free access / Freeware
View	Converter / Software	BiblioSphere PathwayEdition	BiblioSphere	URI	Purchase required
View	Database / Data file	BioCyc Database Collection	BioCyc	URI	Different License Types
View	File format	Biological Pathways Exchange	BioPAX	URI	Open access / Open source
View	File format	Biological Pathways Exchange Level 1	BioPAX Level 1	URI	Open access / Open source
View	File format	Biological Pathways Exchange Level 2	BioPAX Level 2	URI	Open access / Open source
View	Database / Data file	BioModels Database	BioModels	URI	Open access / Open source
View	Database / Data file	Biomolecular Object Network Databank	BOND	URI	Free after registration
View	Database / Data file	bioPIXIE (yeast)	bioPIXIE	URI	Unknown
View	Converter / Software	BioUML - framework for systems biology (probably discontinued)	BioUML	URI	Open access / Open source
View	File format	CellML language	CellML	URI	Open access / Open source
View	Database / Data file	CellML Model Repository	CellML MR	URI	Free access / Freeware
View	Converter / Software	CellML2SBML	CellML2SBML	URI	Open access / Open source

Figure 5: Search entries of BiNCo-wiki. On the left side the search form and on the right side the results are shown. The initial setting shows all entries.

a user is able to log in the account has to be activated using a key sent to the email address.

Create an entry To create a new entry the user must click on the link on the home page or the button on the “List of all BiNCo entries” page. The provided form allows the input of the main information. Additional information such as Java Web Start applications or source code snippets has to be inserted after the creation of the entry.

Create a connection A new connection can be created in different ways. For example, on the “List of all BiNCo Entries” page there is a “Create new link” button. Using this button the user is able to choose a source and a sink entry for the link and to enter a connection type and a description.

Create an application To add a Java Web Start application in BiNCo-wiki there must be an existing software entry. On the Edit page of this entry there is the possibility to add JAR files. These files are available for download. Additionally there is the option to group multiple JAR files to JNLP file. This Java Web Start application file allows the launch of applications directly from the internet. The link to this JNLP file is available on the “View entry” page.

Request edition A user is not able to add or correct information in an entry where he is not the owner. Using the “Request edition” button there is an option to request administrators and the owner of the entry to edit the information or to delete the entry.

Browse history There is a history available for all edited entries. To view the history there is a button on the “View entry” page.

4 Application Example

The following two scenarios show how BiNCo-wiki can be used.

4.1 Scenario 1 - Finding information in BiNCo-wiki to visualize a network

A researcher interested in metabolism would like to analyze a metabolic pathway, for example, the tricarboxylic acid (TCA) cycle of *Escherichia coli* as given by the pathway database KEGG [11]. An image of this pathway can be seen on the KEGG web site (see Fig. 6), but the researcher wants to edit the data with his local software for further investigation.

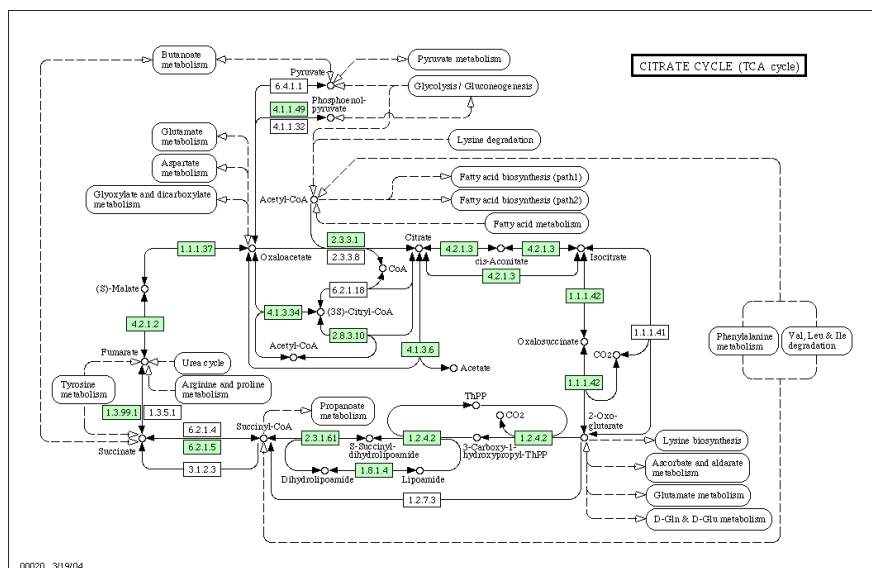


Figure 6: A visualisation of the tricarboxylic acid (TCA) cycle of *Escherichia coli* from the KEGG website [11].

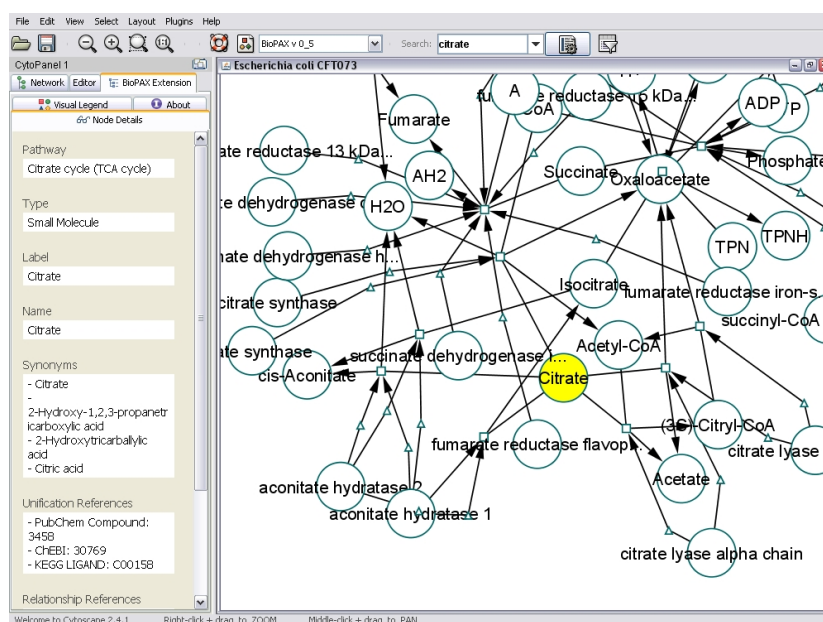


Figure 7: A visualisation of the TCA cycle of *Escherichia coli* in Cytoscape [18].

In BiNCo-wiki each visitor is able to obtain information on the available export formats of KEGG. On the page that displays the KEGG entry a connection to *BioPAX Level 1* labeled “Exports” is shown. Also the URI to the export page is provided in the description of this connection. Knowing this, the visitor is now able to obtain the file `ecc00020.owl` in the *BioPAX Level 1* format. Following the link in the connection the entry of *BioPAX Level 1* is

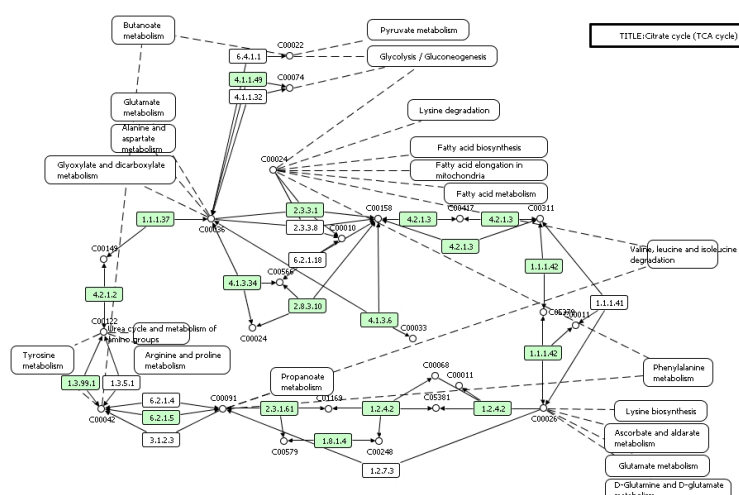


Figure 8: The TCA cycle of *Escherichia coli* visualized in VANTED [10].

shown. Here is a link pointing to the more general description of *BioPAX* [1]. On the page for *BioPAX* a connection to *Cytoscape* [18] with the description “Cytoscape is capable to import files in the BioPAX format.” is presented. Using *Cytoscape*, the .owl file can be imported and displayed as shown in Fig. 7.

An alternative way to visualize the data is using the export format *KGML* [12] and the software *VANTED* [10]. This option can also be found using the connections available in BiNCo-wiki. The result is shown in Fig. 8.

4.2 Scenario 2 - Finding information to convert a network file into another file format

A visitor would like to convert a BioPAX [1] file to a GML [9] file. To view the software that is able to read BioPAX files the visitor has to visit the entry page of BioPAX. On this page the software Cytoscape is shown. Following the link to the information page of Cytoscape the visitor is able to see that Cytoscape is capable of exporting files in GML format.

5 Discussion

To collect and investigate biological network data from different data sources several approaches are possible: collections of links to databases (e. g. Pathguide [3], SRS [6]), mediator and workflow systems accessing data sources by reformulating user queries into data source-specific queries (e. g. DiscoveryLink [8], Taverna [15]), and data warehouses integrating data sources in one new database (e. g. cPath [4], ONDEX [13]). Here we focus on the first approach, the collection of information without data integration. A clear advantage of BiNCo-wiki compared to other systems presenting information about biological network databases and related information is the wiki character. It allows all users to keep the information up-to-date and insert information on new objects without the burden to implement adapters or being responsible for data conversation. Another advantage of BiNCo-wiki is the possibility of linking entries by using connections. The connections represent the linking of different objects. They can be used

to find information on related objects. Related objects can be export formats available for data sources, data sources with similar data, or software applications that are able to import data from this database. Every link is directed and contains an action that describes this link. Being able to find the matching software by using connections of BiNCo-wiki makes data analysis easier.

BiNCo-wiki is different to several other collections of network databases such as Pathguide and the Nucleic Acids Research database. Pathguide is a collection of more than 200 biological pathway resources. The web interface is available at <http://pathguide.org>. The list is maintained by the Bader lab [3]. The resources are assorted in the following overlapping groups: protein-protein interactions, metabolic pathways, signaling pathways, pathway diagrams, transcription factors / gene regulatory networks, protein-compound interactions, genetic interaction networks, protein sequence focused, and other. Each entry provides information about databases similar to the information in BiNCo-wiki. In addition, in Pathguide a ranking of the databases related to Googles PageRank is provided. PageRank is a measurement of the linkage between web sites to estimate the importance of web sites [16]. The resources can be sorted by name or by web popularity. Filters allow subsets of the list such as organisms, availability (license) and standards (export standards) to be shown. The Pathguide listing is manually curated. To change information an email has to be sent to the authors. This method needs staff to keep Pathguide up to date and to answer the emails. Another function of BiNCo-wiki that does not exist in Pathguide is the linkage of entries. For some databases Pathguide shows export types, but no further information on these types is provided. Another system is the Nucleic Acids Research database, a well categorized list of various data sources presented in special issues of *Nucleic Acids Research* [7]. Currently, more than 900 data sources are listed. However, only a small part of these data sources is related to pathways or networks. This collection is also manually curated. Every entry consists of the following fields: the name of the data source, the URI to the web site, the authors of the publication in NAR, a contact email address, a description of the database, acknowledgments, and a link to the NAR publication.

Two tools related to BiNCo-wiki are BioNetBuilder and cPath. BioNetBuilder [2] is a plugin for Cytoscape. It allows the import of data directly from databases and the combination of information from different databases. Currently the following databases are supported: DIP, BIND, Prolinks, KEGG, HPRD, The BioGrid, and GO. Similar to Pathguide and NAR, the plugin does not allow the addition of new data sources. cPath is an open source database and web application for collecting, storing and querying biological pathways [4]. As import formats the Proteomics Standards Initiative Molecular Interaction and the Biological Pathways Exchange XML formats are available. The cPath server software also allows the export of data in these formats via a web interface. In contrast to BiNCo-wiki, cPath is not a collection of available data sources, but it is a server software that is able to collect data, to store it in the underlying database and to make it available via the web interface. The cPath plugin available for Cytoscape uses this web interface to receive data stored in the cPath demo server at <http://cbio.mskcc.org/cpath>.

The integration of the provided information into a workflow system, for example Taverna [15] would be a benefit for users of BiNCo-wiki. For that each database has to be modeled as a data source providing information about networks, network analysis tools have to be modeled as data sinks and links and converters have to be modeled as mediators which connect, either without modifications or with the required transformations, the network information provided by the databases to the requested analysis tools. To achieve this goal it is necessary that databases

holding network information are addressable as web services. Currently this is the case for only a few of the network databases referenced in BiNCo-wiki.

6 Conclusion

We presented a wiki system called BiNCo-wiki. It is a collection of data sources for biological networks, file formats that save/exchange biological networks, and software to analyze the information of these sources. In contrast to existing collections of biological networks BiNCo-wiki presents not only data sources but also related tools, and furthermore allows all users to add and modify information.

An initial content of the system with 51 entries and 56 connections is provided. The available entries are sufficient to present the features, but they do not show the full potential of BiNCo-wiki. Like other wiki systems the collaboration of all users will improve and extend the content of BiNCo-wiki. The more users work with BiNCo-wiki, the more information will be inserted. The wiki character enables all users to update incorrect and insert missing information.

We invite everybody interested in the analysis of biological networks to browse, search and potentially extend BiNCo-wiki!

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