

MEMOSys

Installation Description

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Contents

1	Introduction	3
1.1	MEMOSys	3
2	Requirements	4
2.1	Hardware requirements	4
2.2	Software requirements	4
2.2.1	LibSBML	4
3	Instructions	5
3.1	Download and unpack	5
3.2	LibSBML	5
3.2.1	Linux	5
3.2.2	Windows	5
3.3	PostgreSQL installation	6
3.3.1	Create two new users	6
3.3.2	Create databases and grant privileges	6
3.3.3	Insert necessary values into the Usermanagement database	6
3.3.4	Configure system for correct database (Can be skipped)	6
3.4	Start system	6
3.4.1	Start and test Usermanagement	6
3.4.2	Start and test MEMOSys	7
3.5	Additional Settings	7

1 Introduction

This document describes step by step an installation of the MEMOSys application.

1.1 MEMOSys

The overall goal of systems biology is the simultaneous study of all processes and dynamic interactions at molecular level in order to draw conclusions which may not be apparent when only individual components are considered. Genome-scale modeling is a promising approach to systematically analyze complex cellular systems. Metabolic models have proven to be valuable for increasing the product yield, predicting the effect of gene deletions, improving gene annotation, and identifying regulatory mechanisms. As models are constructed based on annotated genomes, current advancements in next generation sequencing technologies will foster the development of new models.

Therefore, a bioinformatics platform for the management, storage, and development of metabolic models has been established. The web based Metabolic Model System (MEMOSys) supports the development of new models by providing a built in version control system which offers access to the complete reconstruction history. Moreover, the integrated web board, the fine-grained authorization system, and the definition of user roles allow collaborations across departments and universities. Research on existing models is facilitated by a powerful search system, references to external databases, and a feature-rich comparison mechanism. MEMOSys provides customizable data exchange mechanisms using the SBML format to enable analysis in external tools. The web application is based on the Java EE framework and offers an intuitive user interface. It currently contains several well annotated and publicly available models.

In summary, the implemented bioinformatics platform provides researchers a novel application facilitating the management and development of metabolic models.

2 Requirements

This document provides an installation instruction for the web server MEMOSys. Currently it is hosted on the [ICBI Server](#) (Innsbruck Medical University).

2.1 Hardware requirements

Server with at least 1 GBytes of main memory

2.2 Software requirements

- PostgreSQL 8.x.x (alternatively Oracle)
- Java JDK 1.6.x
- Be sure that JAVA_HOME points to your JDK installation

2.2.1 LibSBML

MEMOSys uses a modified version of libsbml to parse SBML files. The instructions for configuration are provided at 3.2.

3 Instructions

The whole system consists of two components which can run independently on different machines:

- **Usermanagement System:** provides the central usermanagement and manages its access rights
- **MEMOSys:** the core application

Security: The communication between the components is based on http connections which should be secured by SSL layer security (HTTPS).

3.1 Download and unpack

Download MEMOSys from <http://www.icbi.at/MEMOSys> (Download tab) and unpack `memosys.zip`.

3.2 LibSBML

3.2.1 Linux

1. Go to `libsaml`
2. Call `./configure --with-java=<INSERT JAVA> --prefix=<INSERT DIR>/libsamlbin`
–insert the directory of your java installation and replace current install dir–
(e.g.: `./configure --with-java=/opt/jdk --prefix=/home/stephan/tempMEMOSys/libsamlbin`)
3. Call `make`
4. Call `make install`

3.2.2 Windows

Build the project using the provided source (`libsaml` directory). Detailed instructions can be found [here](#). However, currently we do not provide active support for Windows installations.

3.3 PostgreSQL installation

3.3.1 Create two new users

- MEMOSys (for example)
 - username: memosys
 - password: memosys
- Usermanagement Sysem
 - username: usermanagement
 - password: usermanagement

3.3.2 Create databases and grant privileges

- Create new database called **memosys** (mapping has to be to public)
- Create new database called **usermanagement** (mapping has to be to public)
- Grant the usermanagement user all privileges to the usermanagement database
- Grant the memosys user all privileges to the memosys database

3.3.3 Insert necessary values into the Usermanagement database

Apply the `insertUsermanagementScript.sql` on the **usermanagement** database as user **usermanagement** (important!).

3.3.4 Configure system for correct database (Can be skipped)

If you use PostgreSQL and the above mentioned default settings **no** additional configuration is required. Otherwise change the username and password in

- **MEMOSys:**
adjust `MEMOSys/server/default/deploy/MEMOSys-ds.xml`
- **Usermanagement:**
adjust `Usermanagement/server/usermanagement/deploy/postgres-ds.xml`

3.4 Start system

3.4.1 Start and test Usermanagement

Go to `Usermanagement/bin` and start `run.bat` (Windows) or `run.sh` (Linux).
Linux - if the file is not executable run `chmod +x run.sh`.

Open a web browser and go to <http://localhost:10080/UsermanagementWeb>.

Login as

- username: `admin`
- password: `myadmin!1`

3.4.2 Start and test MEMOSys

Go to MEMOSys/bin and start `run.bat` (Windows) or `run.sh` (Linux).

Linux - if the file is not executable run `chmod +x run.sh`.

Open a web browser and go to <http://localhost:8080/MEMOSys>.

Login as

- username: `demo`
- password: `demo!1`

New users can be created in the Usermanagement system and need to be assigned to the correct group.

3.5 Additional Settings

The directory where files are stored is currently in

MEMOSys/server/default/applicationdata.

You can change this setting by editing the `dataDirectory` in the `serversetting` table (memosys database).

The current port-prefix settings are:

- **MEMOSys:** 80xx (e.g.: 8080)
- **Usermanagement:** 100xx (e.g.: 10080)

To change the settings create/modify the `bindings.xml` file in MEMOSys/server-conf/bindings.xml or Usermanagement/server-conf/bindings.xml.

For linux systems there are two scripts that are used to start/stop the Usermanagement and MEMOSys system.

They are located at the root of the systems:

- Usermanagement - **`init_usermanagement.sh`**
 1. alter `JBOSS_HOME` in this file
 2. if the file is not executable run `chmod +x init_usermanagement.sh`

3. start system with `./init_usermanagement.sh start`
 4. stop system with `./init_usermanagement.sh stop`
 5. log files are in `Usermanagement/log`
- **MEMOSys - `init_memosys.sh`**
 1. alter `JBOSS_HOME` in this file
 2. if the file is not executable run `chmod +x init_memosys.sh`
 3. start system with `./init_memosys.sh start`
 4. stop system with `./init_memosys.sh stop`
 5. log files are in `MEMOSys/log`