

TINTIN (Target-based Signaling Network Similarity Computation)

USER GUIDE (Version 1.0)

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1. TINTIN Installation

TINTIN uses several other publicly available tools and software for pre-processing files and storing data. In particular, the PostgreSQL database management system is used for storing data and R is used for computing statistical test results. PostgreSQL and R (together with the listed packages) have to be installed in order for TINTIN to function. Please adhere to the recommended version as it has been tested. Note that TINTIN has been tested for installation on the Windows 7 Professional platform.

1.1 PostgreSQL 9.3

Installing PostgreSQL 9.3

Step 1: Download and install PostgreSQL v9.3.x from <http://www.postgresql.org/>.

Please refer to <http://www.postgresqltutorial.com/install-postgresql/> for additional guidance on installation using the PostgreSQL installer for Windows.

Step 2: During the setup progress, when prompted for password (Fig.1), type in “tintin”.

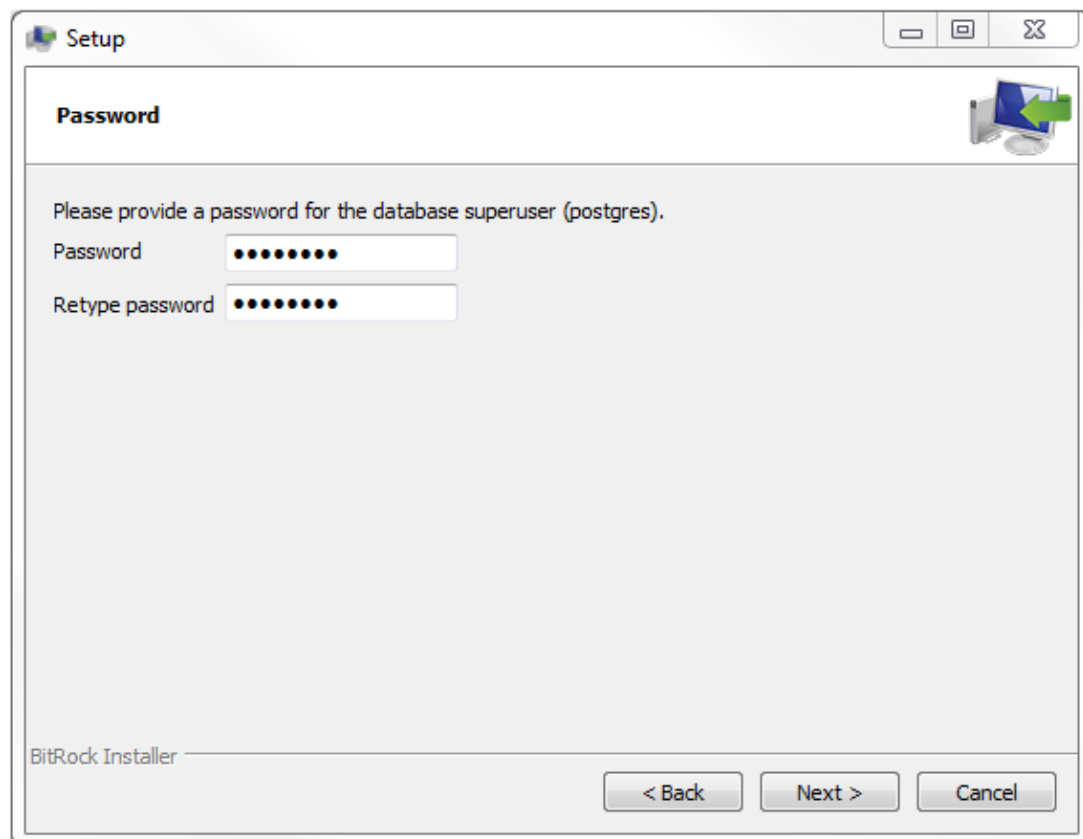


Fig. 1: Password prompt during PostgreSQL installation on Windows.

Verifying the installation

Step 3: Select “pgAdmin III” from programs to launch PostgreSQL (Fig. 2)

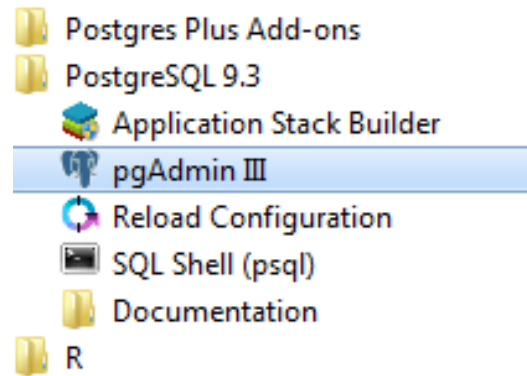


Fig. 2: Launching PostgreSQL

Step 4: Double click on PostgreSQL 9.3 on the object browser and enter “tintin” as the password when prompted (Fig. 3).

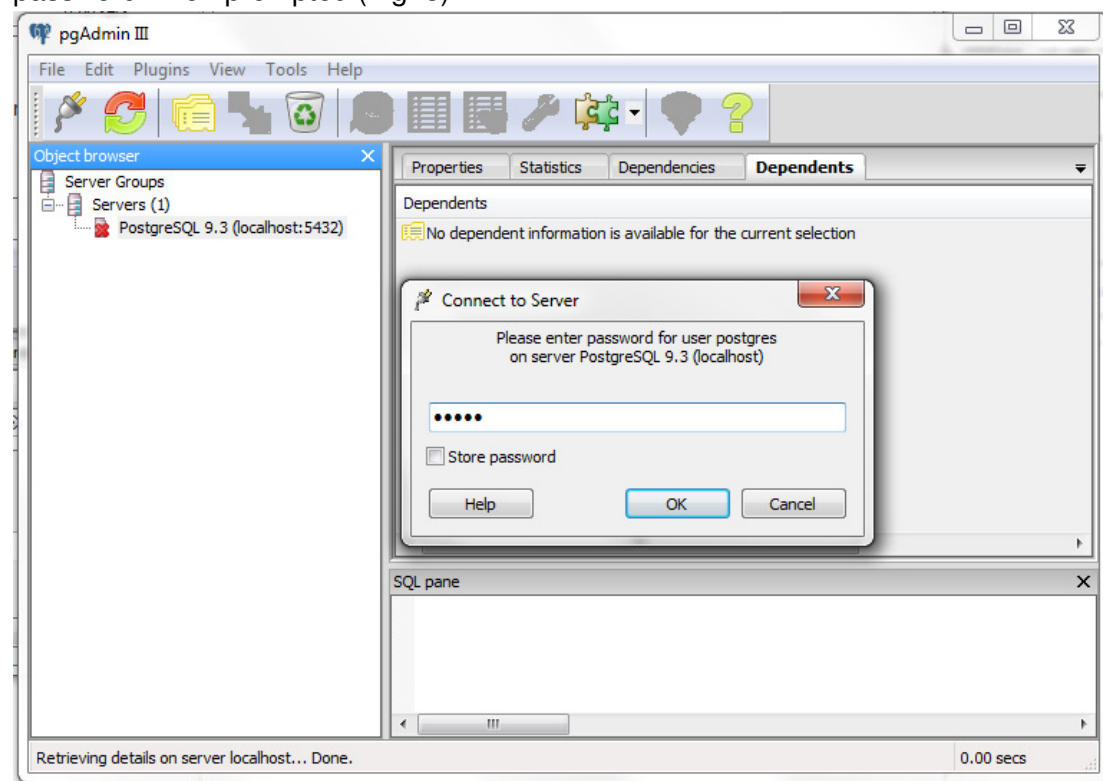


Fig. 3: Connecting to PostgreSQL server

Creating the TINTIN database

The TINTIN database is used by TINTIN for storing data and has to be created before running TINTIN. The database creation has to be done only once during the installation phase and will be available subsequently when TINTIN is run.

Step 5: Right-click on “Databases” on the object browser and select “New Database...” (Fig. 4)

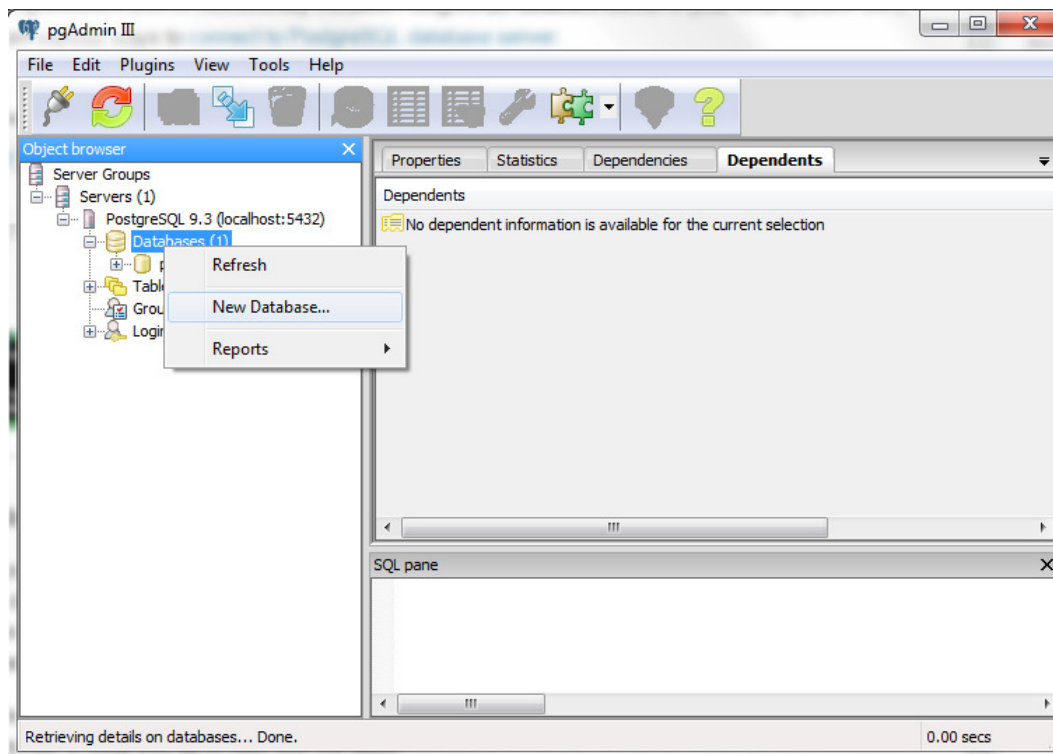


Fig. 4: Creating new database

Step 6: Type in “TINTIN” as the name of the database (Fig. 5) and select “OK”.

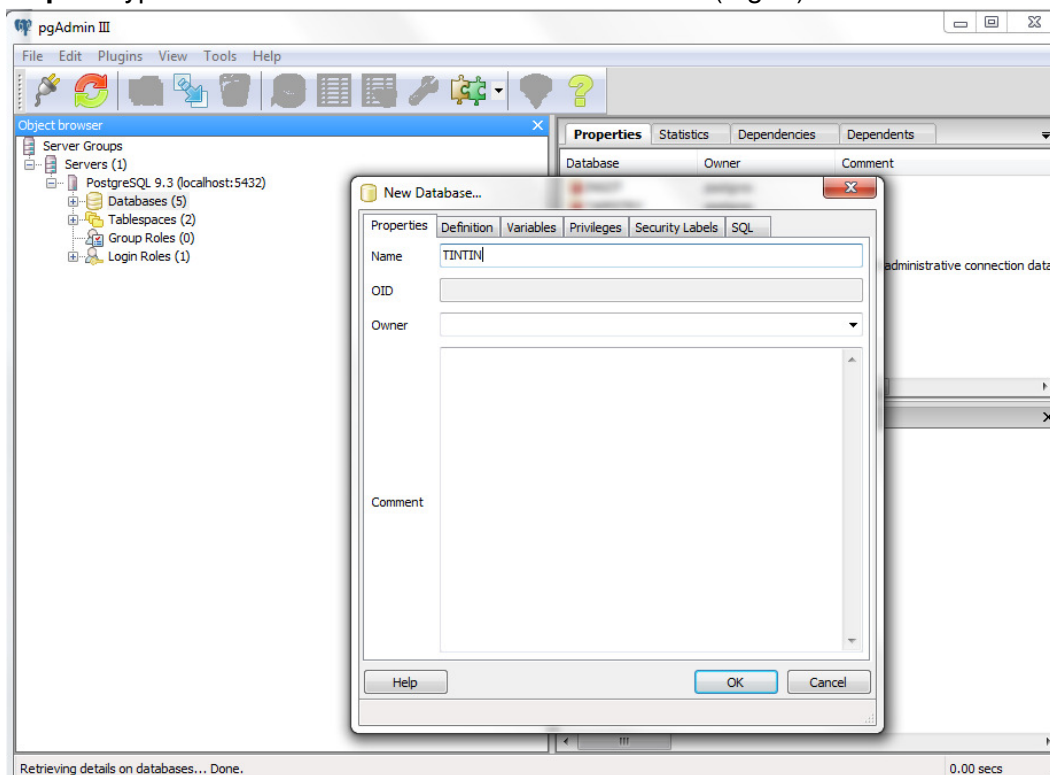


Fig. 5: Setting the name of the new database

Step 7: Verify that the “TINTIN” database has been created

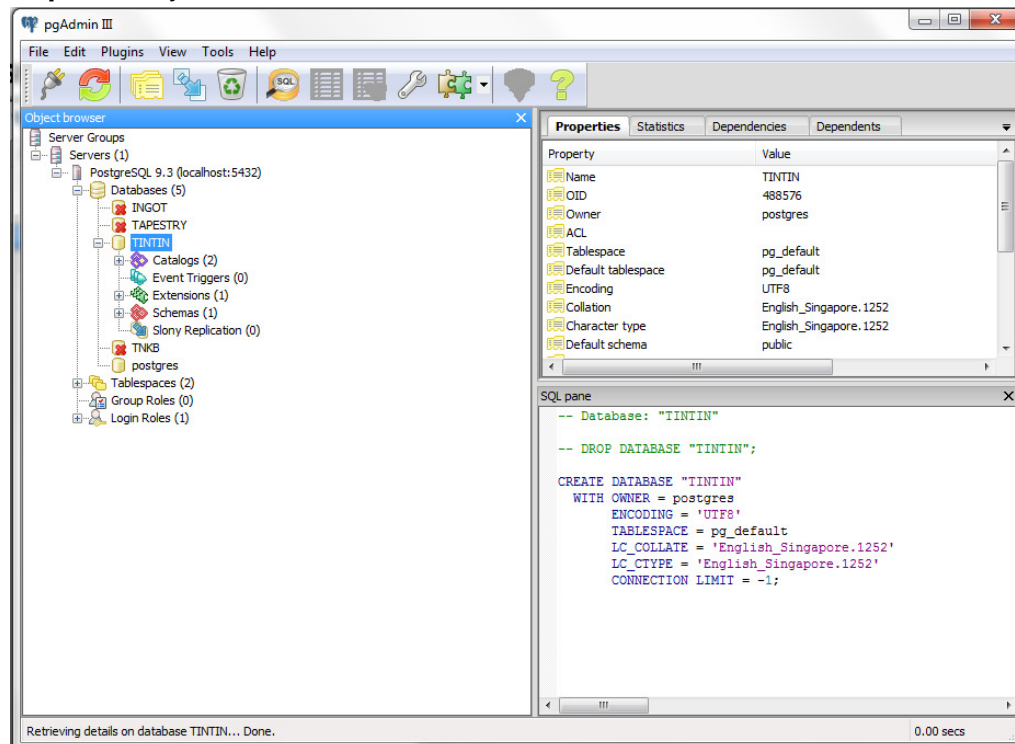


Fig. 6: Verify that the new database has been created

1.2 R 3.1.2

Step 1: Install R version 3.1.2.

Step 2: Install and load the following packages

- Rserve
- survcomp (installation instruction for survcomp can be found at <http://www.bioconductor.org/packages/release/bioc/html/survcomp.html>)

1.3 network_lib_TINTIN folder

This folder contains the example files for running TINTIN.

TINTIN requires several files from this folder for proper execution:

1. featureLib_list.txt
 - contains the list of files (e.g., hatakeyama2003_MAPK_features.xlsx) containing the feature values of the training networks used by TINTIN for target prioritization.
 - contains the list of files (e.g., hatakeyama2003_MAPK_model.dat) containing the SVM regression model of the training networks (generated by TENET).
 - contains the list of predictive topological features of the training networks.
2. <trainingNetwork>_timeseries.dat

– contains the time series data for computing the PSSD feature. The data in this folder are generated by Copasi using the .sbml file of the training network as inputs.

3. <signalingNetwork>.xml

– contains the signalling network model that is described in SBML format. An example is Hatakeyama2003_MAPK.xml. The BioModels repository (<http://www.ebi.ac.uk/biomodels-main/>) provides signalling networks that are described in the SBML format.

Step 8: Copy the “network_lib_TINTIN” folder to the C directory “C:\” (Fig. 7)

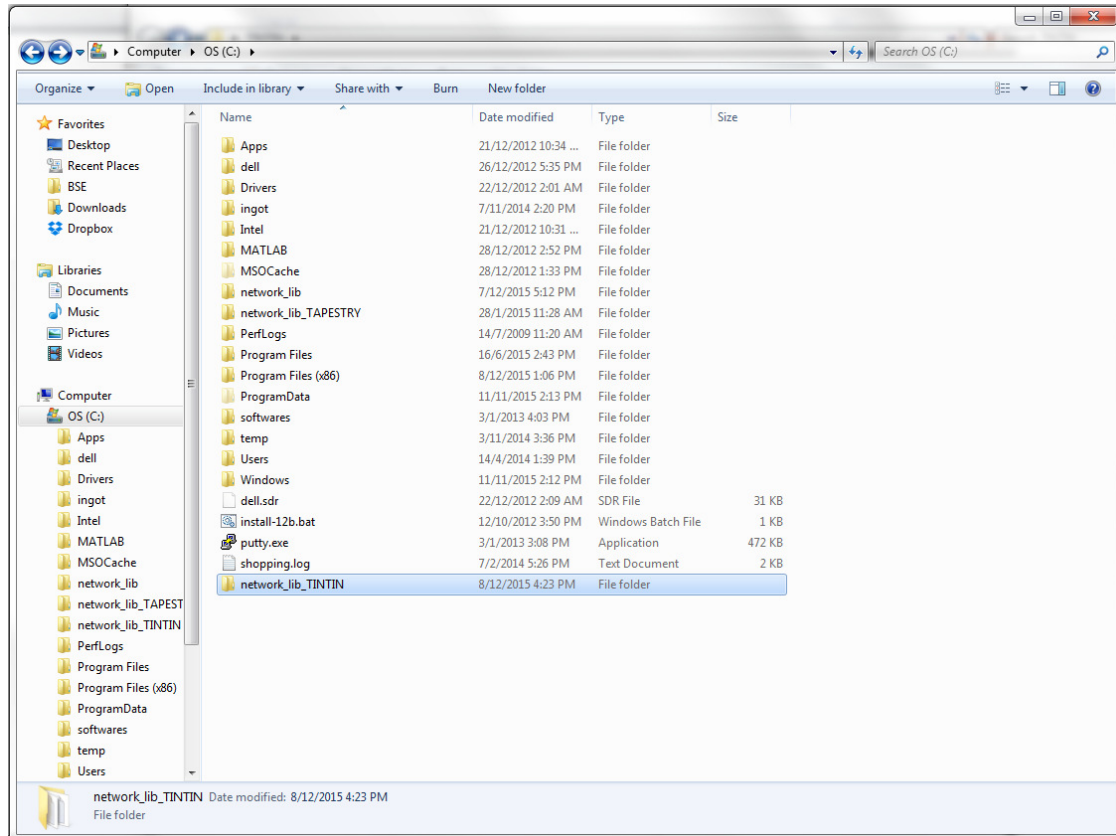


Fig. 7: Copy “network_lib_TINTIN” folder to C directory

1.4 TINTIN.jar

Step 9: Copy TINTIN.jar to a desired location (e.g., “C:\Desktop”).

2. Launching TINTIN

Step 1: Start Rserve from R (Fig. 8).

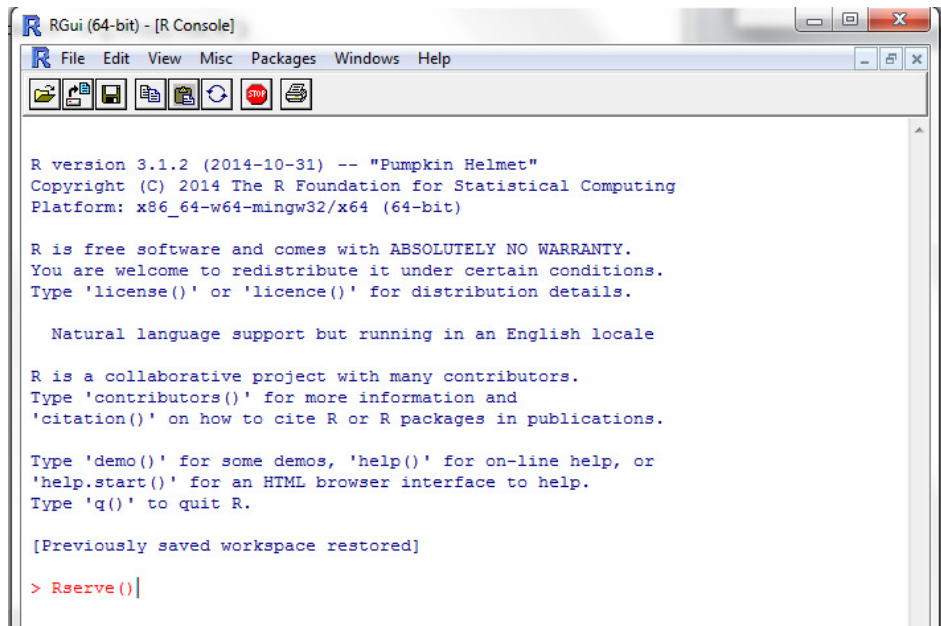


Fig. 8: Start Rserve

Step 2: Launch command prompt dialog (cmd.exe) (Fig. 9).

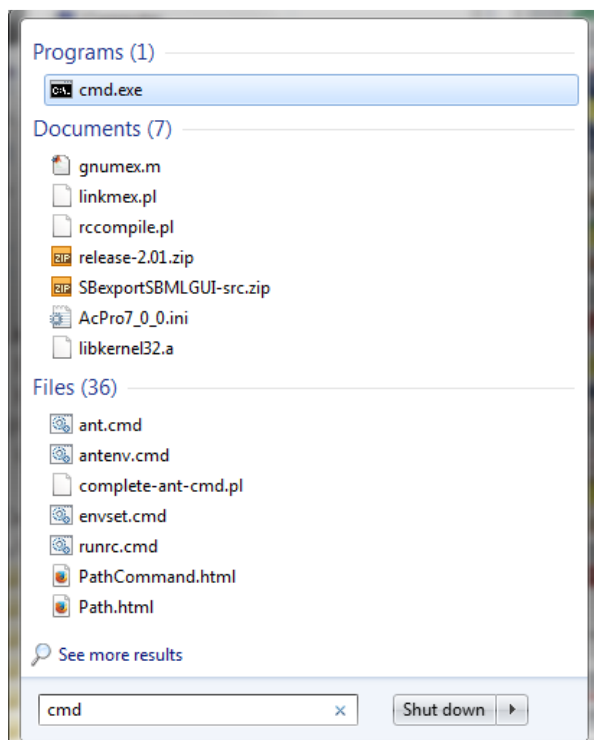
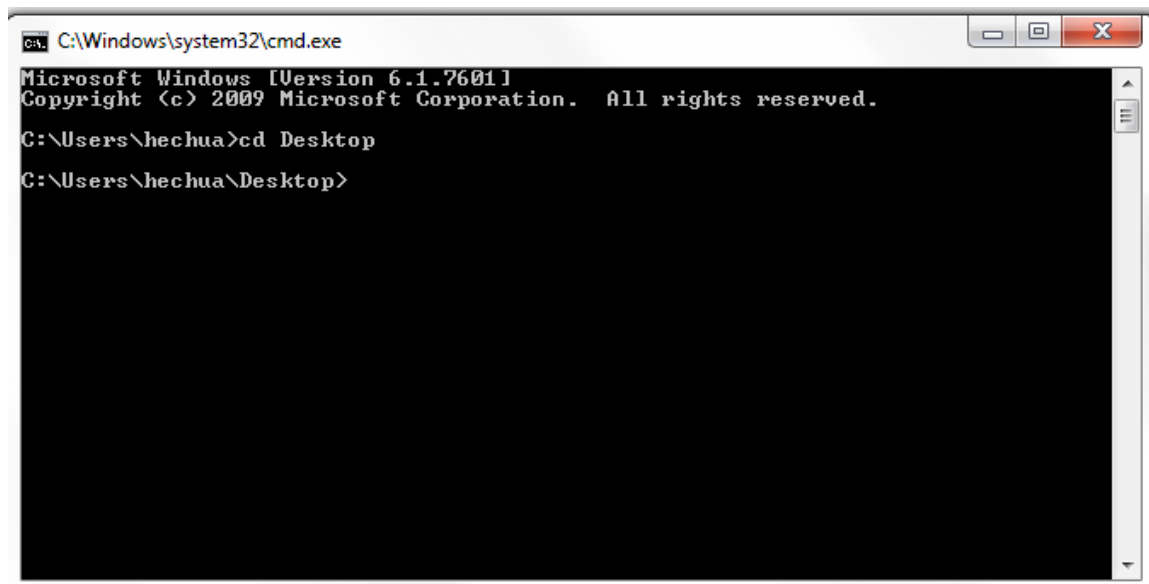


Fig. 9: Launch cmd.exe

Step 3: Change the directory to the one that contains TINTIN.jar (Fig. 10).

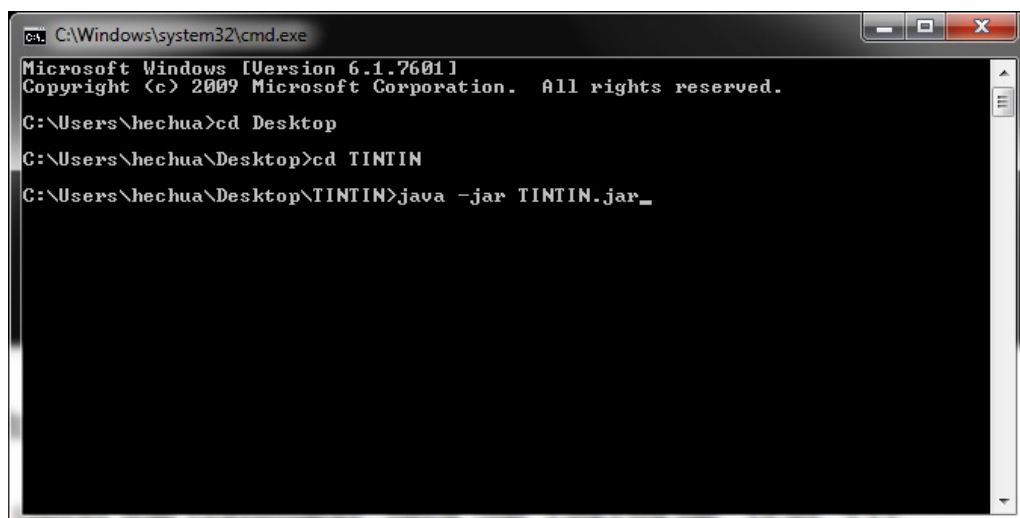


```
C:\Windows\system32\cmd.exe
Microsoft Windows [Version 6.1.7601]
Copyright (c) 2009 Microsoft Corporation. All rights reserved.

C:\Users\hechua>cd Desktop
C:\Users\hechua\Desktop>
```

Fig. 10: Set to the directory containing TINTIN.jar

Step 4: Run TINTIN by using the command “java -jar TINTIN.jar” (Fig. 11).



```
C:\Windows\system32\cmd.exe
Microsoft Windows [Version 6.1.7601]
Copyright (c) 2009 Microsoft Corporation. All rights reserved.

C:\Users\hechua>cd Desktop
C:\Users\hechua\Desktop>cd TINTIN
C:\Users\hechua\Desktop\TINTIN>java -jar TINTIN.jar_
```

Fig. 11: Run TINTIN

3. Using TINTIN

Step 1: Select the input signalling network (Fig. 12).

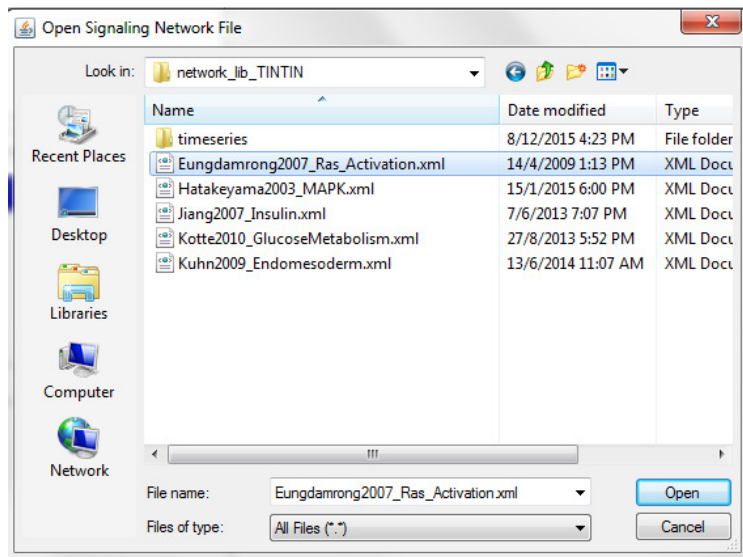
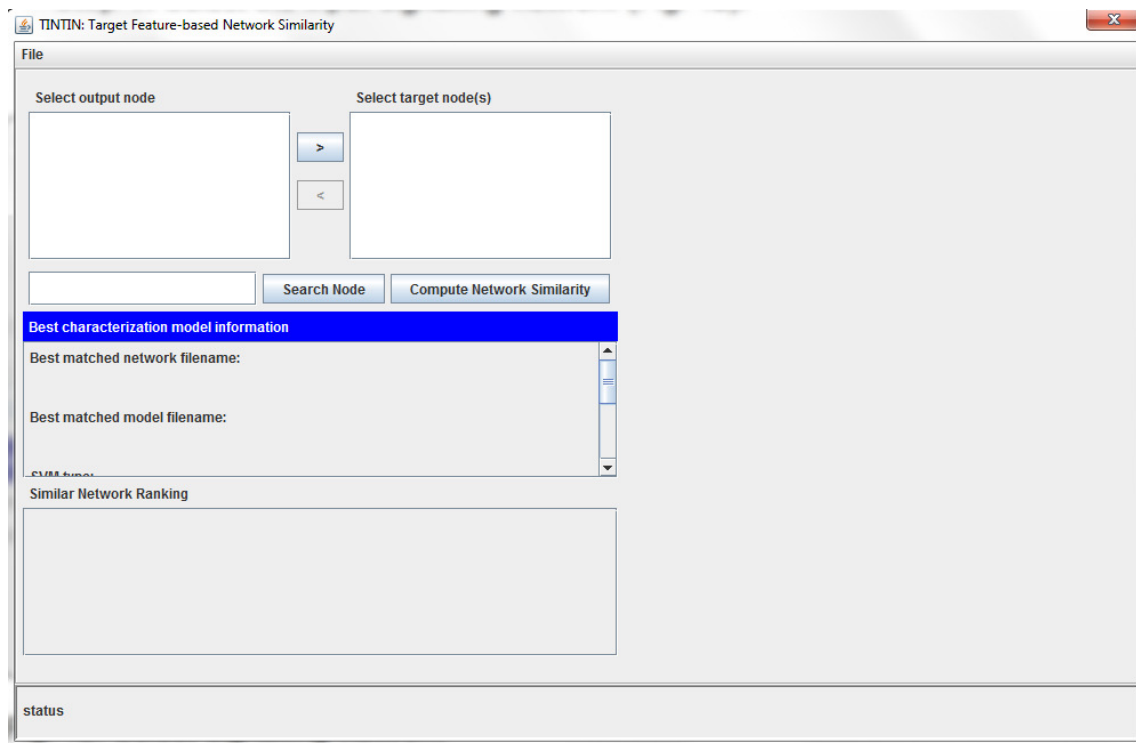


Fig. 12: Select signalling network

Step 2: Select the target node(s) of the input signalling network (Fig. 13).

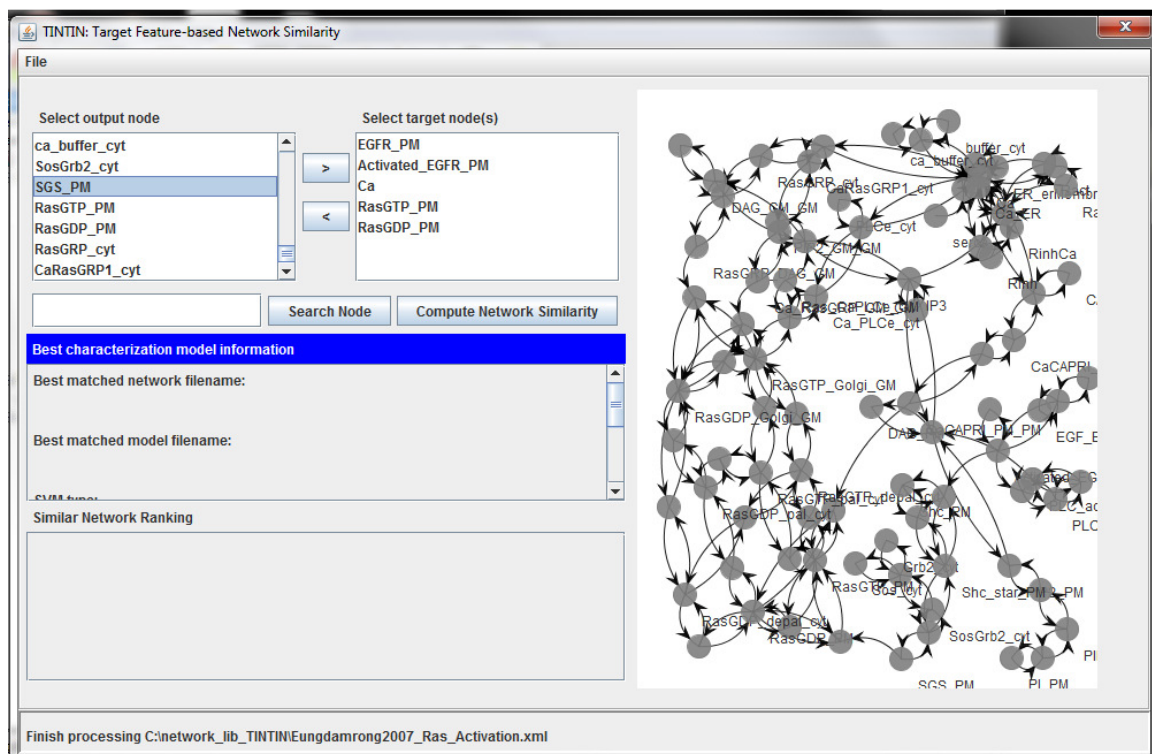


Fig. 13: Select target node(s) for the signalling network

Step 2: Select the output node of the input signalling network (Fig. 13).

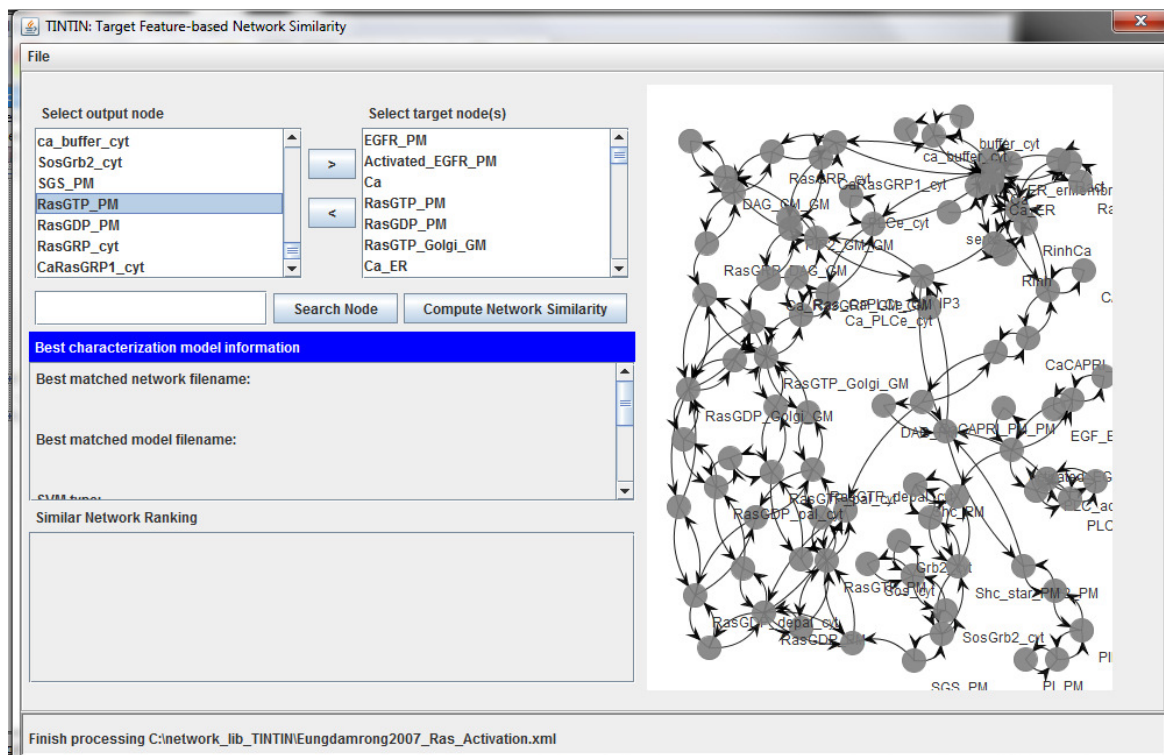


Fig. 13: Select output node for the signalling network

Step 3: Configure network similarity computation task by clicking on “Compute Network Similarity” button and compute similarity by clicking on “Compute Similiarity” button in “Configure Network Similarity Computation Task” dialog (Fig. 14).

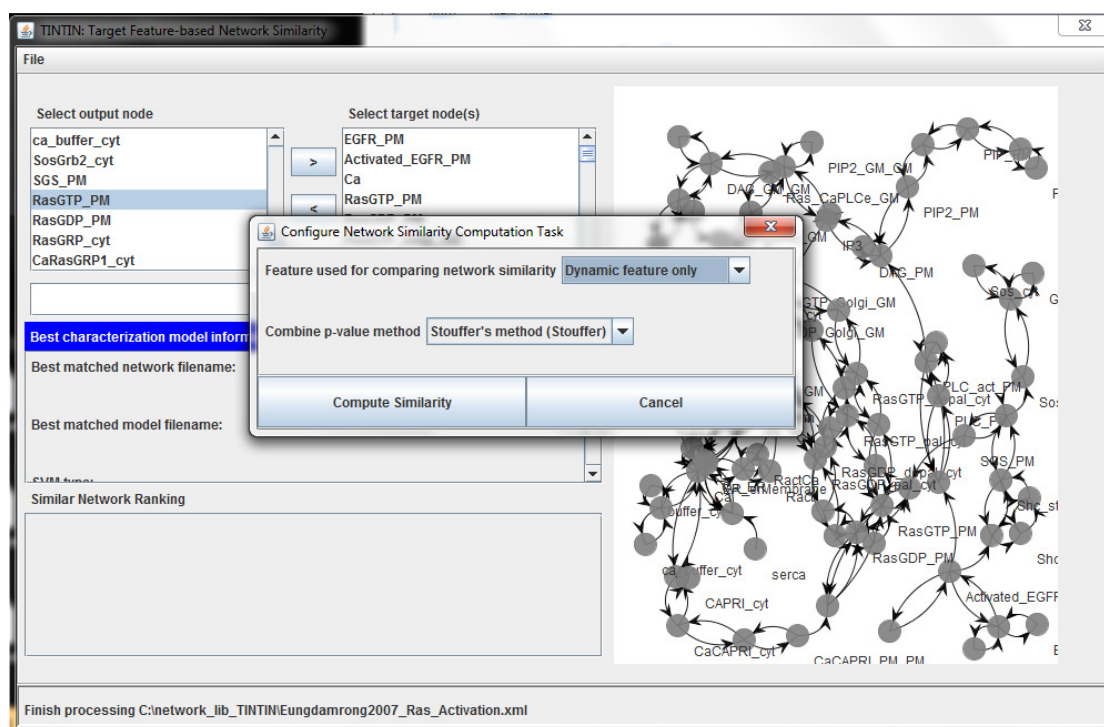


Fig. 14: Perform network similarity computation for the signalling network

Step 4: View network similarity results (Fig. 15).

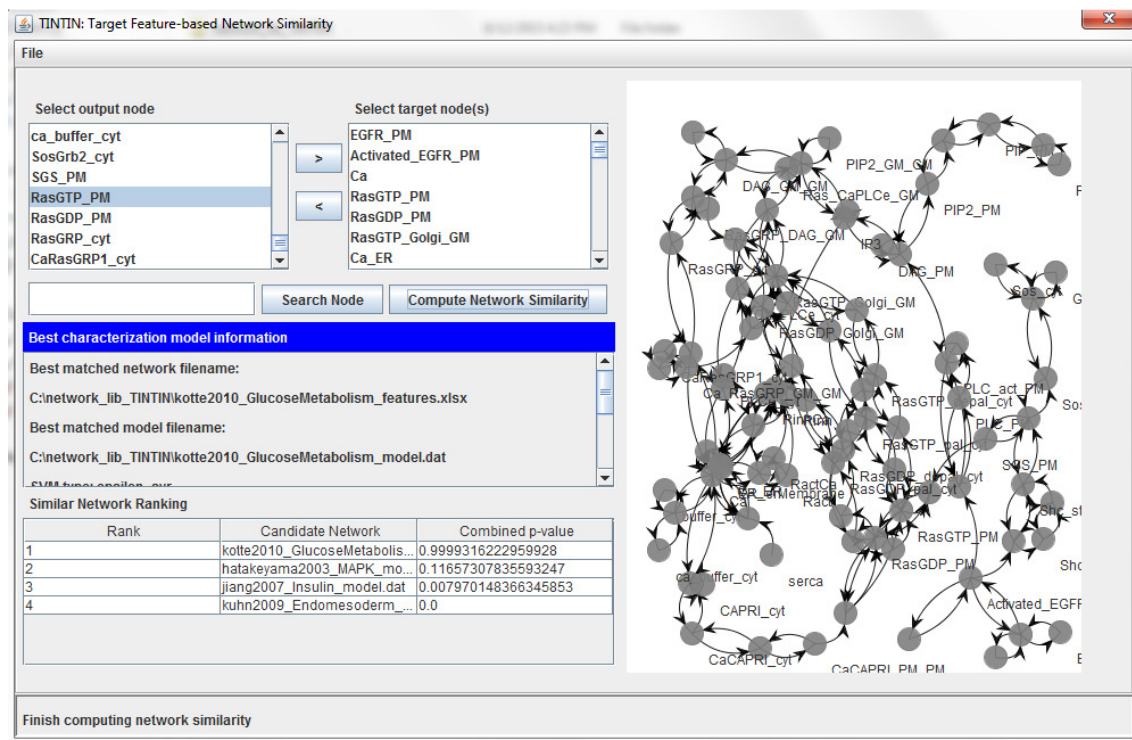


Fig. 15: Displaying network similarity results.

The characterization model of the best matching network is displayed in the “Best characterization model information” panel and the ranking of the candidate networks in the library is displayed in the “Similar Network Ranking” panel.