Scaffold Hunter:

Installation of MySQL and Reconstruction of the profile database as well as a sample database comprising the pyruvate kinase data from PubChem

By Stefan Wetzel

1. Installation of MySQL 5.x

1. Download MySQL Server (Installer) from
   http://dev.mysql.com/downloads/mysql/5.1.html#win32.
   Scaffold Hunter has only been tested with MySQL 5.x.

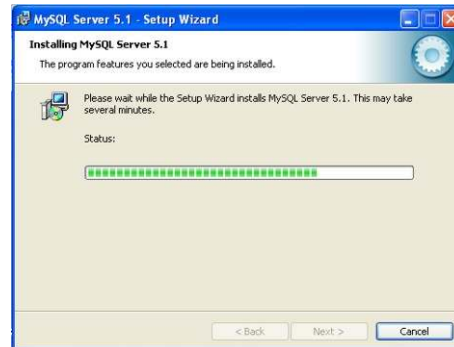2. Execute the installer file and install MySQL

3. Choose "typical"
   If you are an administrator, you may also choose "custom".

4.   Click on "Install"

5.   The installation may take a few minutes.

6.   Click "next".

7.   Uncheck the lower checkbox "Register the
     MySQL server now".
     Click "next".

8.   Click "next".

9. Choose "Standard Configuration".
   Click "next".

10. Click "next".

11. Choose a root password and enter it twice.
    Click "next".

    **Note down this password since it is the
    administrator access to the database!**

12. Click "execute".

13. Click "finish".

The installation described here, sets the default port of the MySQL serve (3306). If you or your administrator chose another port, please use that one in all further steps!

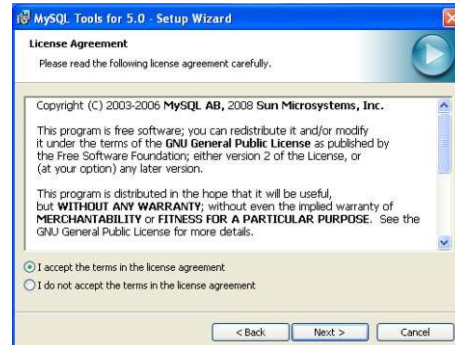Once you have installed the MySQL server, please restart the system.

2. Installation of the MySQL GUI Tools

1. After the installation of the MySQL server, please download the MySQL GUI Tools from the website http://dev.mysql.com/downloads/gui-tools/5.0.html.

2. Execute the installer file and install the MySQL GUI Tools.
    Click "next".

3. Read the license agreement and check "I accept the terms in the license agreement" if you agree with it.
    Click "next".

4. Click "next".

5.   Choose "Complete".
      Click "next".

6.   Click "Install".

7.   The installation may take a few minutes.
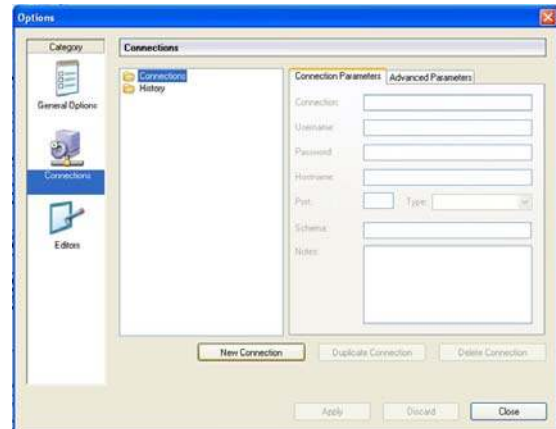
7.   Click "finish".

After the installation, you find the programs in the MySQL folder under Start/Programs.
Please start the "MySQL administrator".

When you first start the MySQL administrator, you need to establish a database connection.
To do so, please follow these steps:
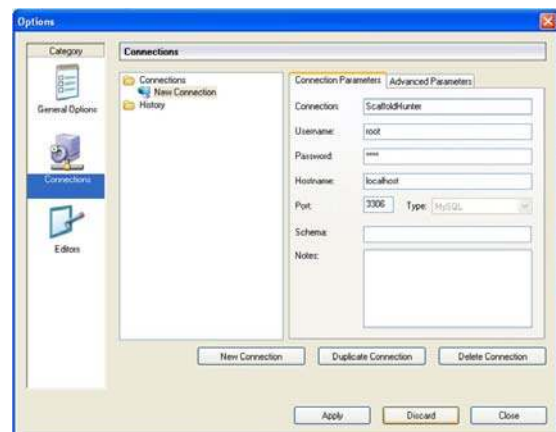
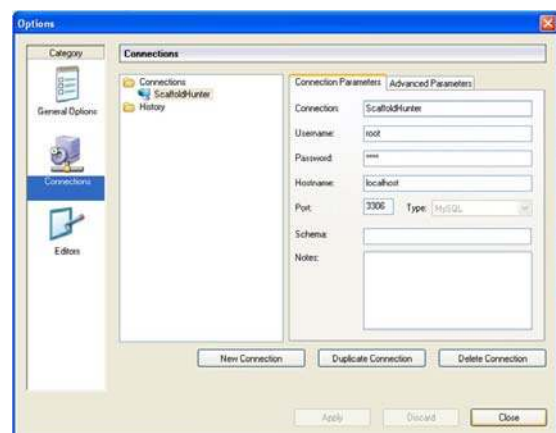1.   Klick on the button with the three dots

2.   chose "new connection" at the bottom of the new
window

3.   enter a name for the connection
enter the username "root"
enter the root password set during the installation
of the MySQL server
if you are running the database on the same
computer, the host is "localhost"
the port should be 3306. Otherwise, please consult
your administrator.
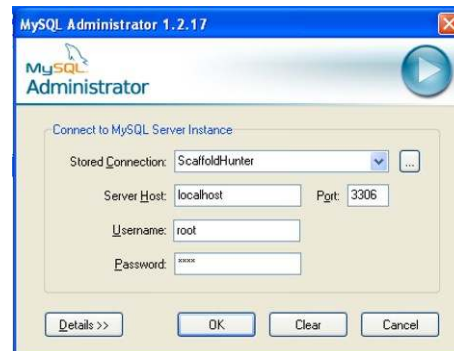Click "Apply".

4.   Click "Close".
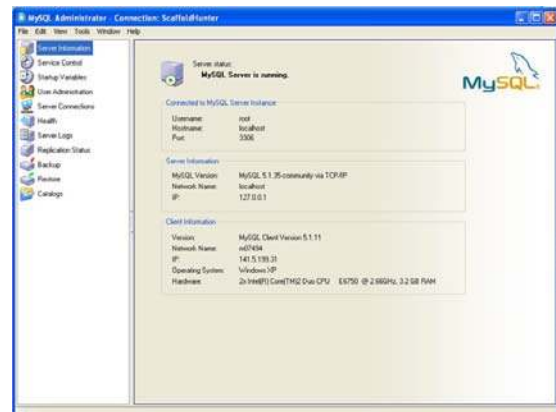
3. Restoring the profile database

The first task is to restore the profile database without which Scaffold Hunter will not work. It will also restore a sample database with the data of the Pyruvate Kinase Screen from PubChem. Both SQL dump files are available as ZIP compressed files from http://edoc.mpg.de/display.epl?mode=doc&id=429252. Please unzip the files before proceeding with this manual. If you do not want to restore the sample database, please stop after step 6 and exit the MySQL Administrator.

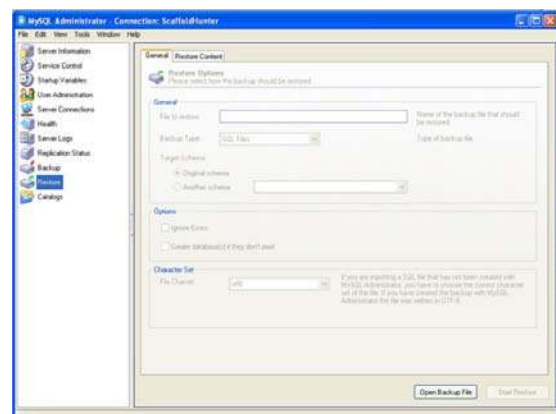Start the MySQL Administrator, then follow the steps given below:

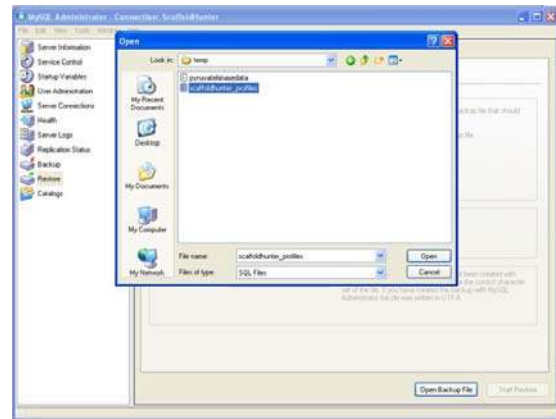|		
1.	For "Stored Connection" choose the connection created before. Click "OK".	
2.	The start screen of the MySQL Administrator looks like that. Choose "Restore" from the items in the frame on the left hand side of the screen.	
3.	Click on "Open Backup File" on the lower right side of the screen.	

4.   Navigate to the folder with the unzipped database
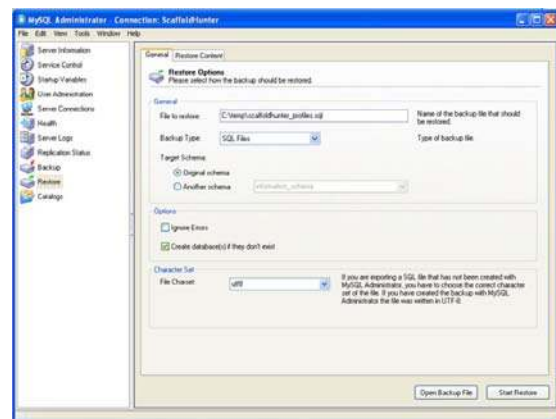   dump files.
     Choose "scaffoldhunter_profiles.sql".
     Click on "open".

5.   Mark "Create database(s) if they don't exist" in
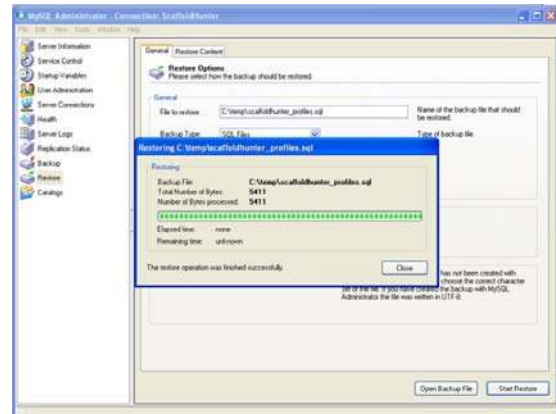   the middle part of the screen.
     Click on "Start Restore".

6.   The restoring of the profiles database is usually
     quite fast (under one minute).
     When it has finished, please close the status bar
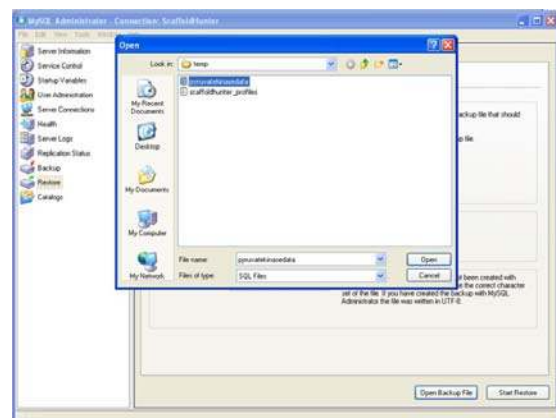   window.

     If the program stops the process with an error
     message, please try again from step 8. If the error
     is repeated, please download the dump file newly
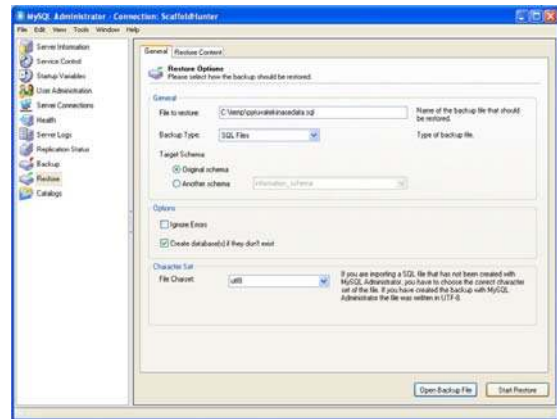   and try again.

7.   If you also want to install the sample database,
     click on "Open Backup File" again.
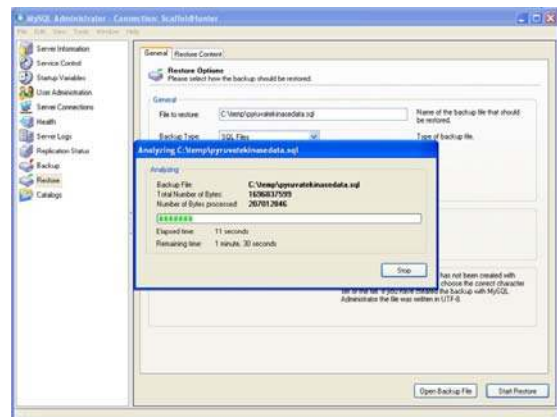   Choose the file "pyruvatekinasedata.sql".
     Click on "Open".

8. Check that "Create database(s) if they don't exist" is still marked. If not, please mark it.
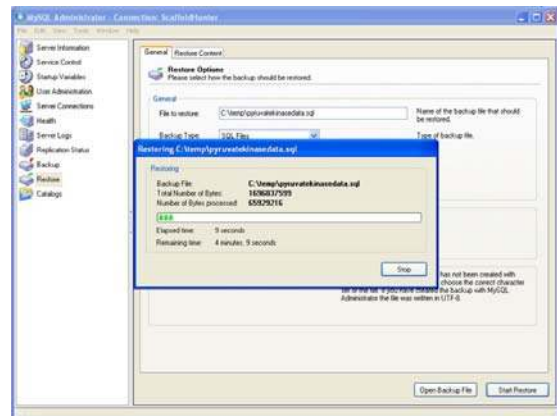Click on "Start Restore".

9. The program checks the integrity of the database. This may take up to 20 minutes and more, depending on your hard- and software.

If the program stops the process with an error message, please try again from step 8. If the error is repeated, please download the dump file newly and try again.

10. After the integrity check, the database will be restored. This may take up to 30 minutes and more, depending on your hard- and software.

If the program stops the process with an error message, please try again from step 8. If the error is repeated, please download the dump file newly and try again.
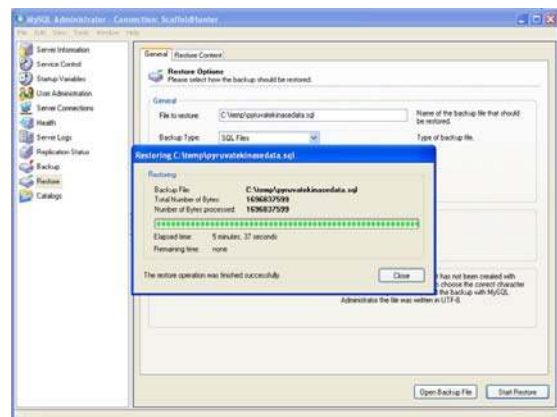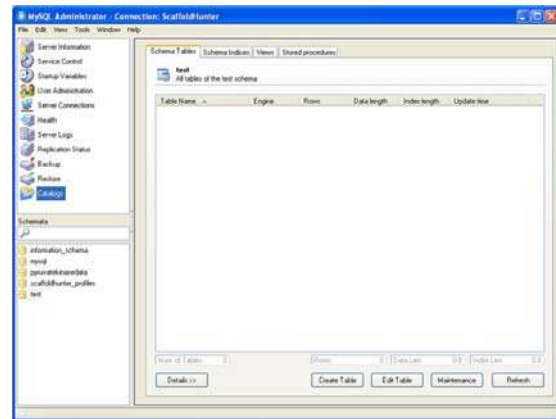

11. Once the restoration of the database is finished, please click on "Close".

12. To check, whether the database have been restored, choose "Catalogs" from the items list on the left hand side of the screen.
All available database are shown in the window underneath the items list, also scaffoldhunter_profiles and pyruvatekinasedata.

5. **Create Scaffold Hunter profile**

On the startup of Scaffold Hunter, choose "Profilverwaltung". Then klick "neues Profil" and you will see the window shown to the right. Choose a profile name – we suggest either you user name or, if you are the only user, the name of the data set. Choose the language and the storage location of the profile.

The standard URL for installations of MySQL with the default settings is already given. If you set another port during the installation of MySQL or have MySQL installed on another computer, please replace "localhost" by the name of the database computer and "3306" by the chosen port number.

Also give the database name (name of the data schema in the MySQL database), the username ("root" if you have not created any other database users) and the corresponding password of the MySQL user. Then click ok.

Now you can start using Scaffold Hunter as described in the manual.