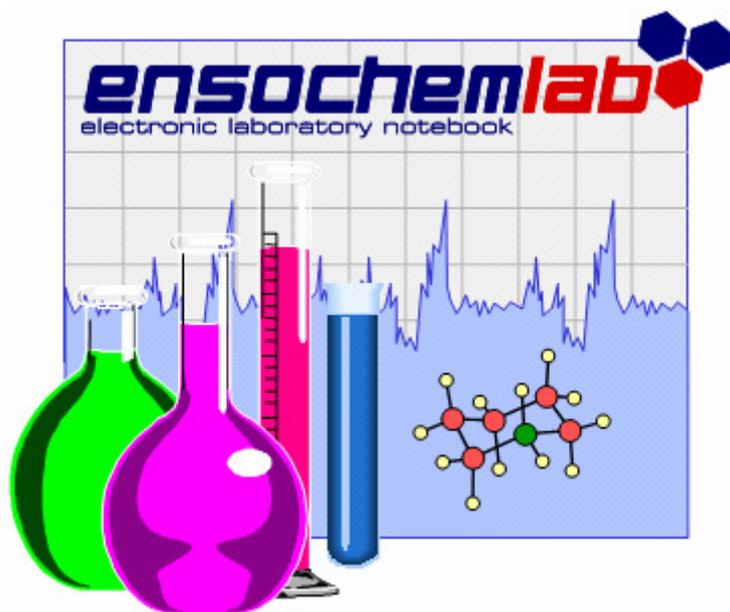


# ensochemLab

Version 6.0

## Installation Guide (Workgroup Edition)



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# 1. Overview

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This guide will lead you through the installation of ensochemLab.

It shows you step by step how to install your software including web server, database and a basic configuration.

The workgroup edition is not intended for a distributed installation. The ensochemLab web server as well as the SQL Server with the database must be installed on a single machine. Access rights can be granted to users in the same domain.

The database system used by ensochemLab workgroup edition is a SQL Server which can be either a "big" server or the slightly limited SQL Server Express which can be downloaded for free from Microsoft's website.

If you have further requirements or need special features not covered by this installation, please contact our experts for advice.

There are some special elements in this guide:

## **Notes:**

You should read them carefully to avoid trouble with your ensochemLab product.

## **Recommendations:**

They help you to use the easiest and most common way through the specific step.

The database setup creates a configuration which provides stability, security and reliability on a very high level.

However, you can change the settings manually after installation if you want to do so. Please note that this is neither recommended nor supported!

Before you begin, you should check that you have full administrator access to a computer running at least Windows 2000 / 2003 / 2008 Server (the edition or type does not matter). Theoretically, you can also ensochemLab on a Windows Workstation computer. However, you are limited to 10 concurrent connections there.

The Internet Information Services (IIS) must always be available started on your server no matter of the operating system.

The SQL Server (or SQL Server Express) must be installed on your server machine.

Most companies have very strict rules for setting up a web server and the required virtual directories. To meet those restrictions this part of the installation must be done manually. This manual lists the necessary steps but does not describe them in details.

On demand, our experts also offer a guided installation or the distribution of preconfigured server systems.

## 2. Preparation

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Before beginning you should make sure that the following components are installed on your Windows 2000 / 2003 or 2008 server:

- Microsoft .NET Framework in version 4.0.
- Internet Information Server
- SQL Server 2005, 2008 or newer (or the respective SQL Server Express versions)

## 3. Web Server Installation

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In an ensochemLab standard installation a web server provides two URLs, one for the ensochemLab server and one for the "ensochemEditor Web Edition" which is a Java applet for drawing chemical structures and reactions.

Most installations use a common virtual directory, i.e. "ensochemLab" and below the directories "ensochemEditor" und "ensochemLabService" which is also the directory structure on the CD in "Server\Server Setup". As a matter of course you can use other descriptions or even a completely different structure. In this case you must adjust the samples from this manual accordingly.

Then copy the folders "ensochemEditor" and "ensochemLabService" from "Server\Server Setup" of the CD into your virtual directory. The folder "ensochemLabService" must be configured as an application on the web server. You must deactivate anonymous access to the virtual directory and allow only integrated Windows authentication.

The files from the folder "CommonFiles" must be copied to a directory which is in the search path of your server.

**Note** If the folder for "CommonFiles" is new or has been newly added to the search path, you should reboot your server to make sure that all system components get to know this path.

You are now able to test your installation very easy with a web browser. If you used different descriptions than recommended you must adjust the URLs accordingly.

### ensochemEditor Web Edition

Enter the URL "<http://localhost/ensochemLab/ensochemEditor/ensochemEditorHelp.htm>". The browser should then display a page with information about ensochemEditor.

### ensochemLab Service

Enter the URL "<http://localhost/ensochemLab/ensochemLabService/Server.aspx>". The browser should display the following error message from the ensochemLab server (maybe in a different format, depending on your browser):

```
<?xml version="1.0" encoding="windows-1252" ?>
- <Application>
- <Error>
  <Module>XMLParser</Module>
  <Function>XMLParser.LoadRequest</Function>
  <Info>Illegal call, request is empty</Info>
  <Computer>BREMEN</Computer>
  <IP>192.168.98.12</IP>
  <System>Win32NT 5.1.2600.196608</System>
  <User>ASPNET</User>
- <Items>
  - <Item>
    <Sender>XMLParser</Sender>
    <Procedure>XMLParser.LoadRequest</Procedure>
    <Message>Illegal call, request is empty</Message>
  </Item>
  - <Item>
    <Sender>Broker</Sender>
    <Procedure>Broker.GetResponseData</Procedure>
    <Message>could not dispatch client's request</Message>
  </Item>
</Items>
</Error>
</Application>
```

Any other error message indicates a problem with your installation. The message may help you to isolate the problem.

# 4. Database Installation

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## *General*

The ensochemLab database consists of objects for chemical reactions and structures as well as objects for alphanumerical data.

The ensochemLab workgroup edition holds both kinds of data in a single database on the ensochemLab server. Data will be accessed in the context of a user's Windows domain account.

An easy to use setup program asks you for required information, installs all objects, loads some administration data and creates the configuration files for running your ensochemLab server.

## ***Preparation***

Before you can start the installation you must create a SQL Server database according to your company rules using an appropriate tool (i.e. SQL Server Management Studio Express).

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## ***Setup Program***

The database installation takes place with the setup program in "Server\Database Setup" on the CD. Just start the program "Setup.exe" on the ensochemLab web server.

The following pages describe the information you must enter for setup.

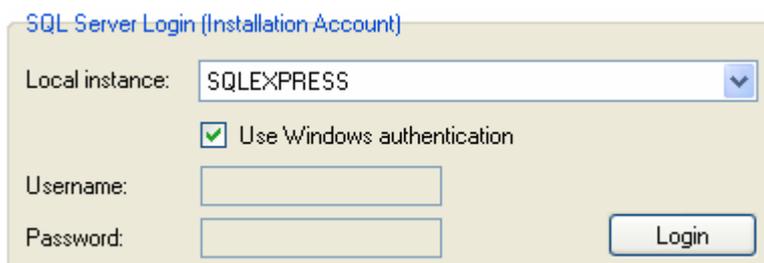
## License Key



The dialog box is titled "ensochemLab License". It contains a text input field for the license key, which is currently filled with "####-####-####-####". Below the input field, the text "Demo license" and "License is valid for 90 days" is displayed.

Enter your license key. Setup will then show additional information about your license. It is possible to accomplish the installation without a license key. However, users can work with ensochemLab as recently as an administrator has entered a valid license.

## Login to SQL Server



The dialog box is titled "SQL Server Login (Installation Account)". It features a dropdown menu for "Local instance:" with "SQLEXPRESS" selected. Below this is a checked checkbox for "Use Windows authentication". There are two text input fields for "Username:" and "Password:". A "Login" button is located to the right of the password field.

If more than one instances of SQL Server are installed on your local server machine, you must choose one of them for installing ensochemLab. Normally you will have only one instance and in this case the selection box is disabled.

If the box "Use Windows authentication" is checked, you will connect to the SQL Server with your Windows account. If you are logged in with administrator rights, this is the recommended mode. In other cases you must enter a user name and a password for the installation account.

Then click "Login" to connect to the database.

## Choose Database



The dialog box is titled "ensochemLab". It contains a dropdown menu for "Database:" with "ensochemLab" selected.

As soon as you are connected to the SQL Server all available database are listed. Please choose the database designated for ensochemLab.

## Paths for Configuration und Protocol

Directories

Logfile directory:  ...

Configuration:  ...

In the upper box you can provide a folder where any database commands and potential errors will be logged. Even if you can perform the installation without a log file, it can give you an important help in case of problems.

In the lower box you can enter the folder where the configuration files of ensochemLab server can be found. If you run setup on the web server the correct directory should be automatically detected.

Using the buttons "... " at the right you can browse for folders.

### Start the Installation

Click on "Start Installation" to perform the installation of the database objects.

## ***Manual Installation***

In addition to the setup program a manual installation is generally also possible even so it is recommended by no means.

**Warning** Manual setup of ensochemLab databases is intended only for very special installations and should only be done in exceptional cases. We strongly recommend performing a manual setup only after consulting our experts.

As with the setup program a manual installation also requires that you first create a database using a suitable tool.

The installation process consists of two parts, creating and initializing the database. All required scripts and a necessary tool can be found on the CD in "Server\Database Setup\Manual Setup".

All scripts must be edited before executing them. Object names contain the placeholder "`<SUFFIX>`" which must be replaced with an appropriate editor by an empty string. For example, "`EC_LAB_MOL_SUB_<SUFFIX>`" must be changed to "`EC_LAB_MOL_SUB`" and "`EC_LAB_RXN_STR_<SUFFIX>_PK`" to "`EC_LAB_RXN_STR_PK`".

After performing a manual installation, the configuration file of the ensochemLab server must be customized and two additional configuration files for accessing the chemistry databases must be created. You will find information about these files in chapter 7.

## Alphanumeric Database

Execute the following scripts in the order stated below:

- Setup Objects.sql
- Load Initial Data.sql

Please note that in these scripts the placeholder "`_<SUFFIX>`" must be replaced as described above.

## Chemistry Database

The objects for chemical data can be created with the script "Create\_Chemistry.sql". In addition to the placeholder "`_<SUFFIX>`" described above this script contains also "`<USER>`". Replace this with the role "EC\_LAB\_READ".

After the script has been executed a set of initial data must be loaded. To do this you must run the command line tool "Substructures.exe". The program must be executed twice from the command line, providing a set of eleven parameters.

## Calling Substructures.exe from the Command Line

(The parameters must be written in one line, divided by blanks. They are listed here one below the other only for better readability)

First call:

```
Substructures MSSQL
              MOL
              ecseSQLServer.dll
              <Server>
              <Database>
              LoginType=WINDOWS
              $$WINAUTH$$
              $$WINAUTH$$
              EC_LAB_MOL_BD
              EC_LAB_MOL_STR
              EC_LAB_MOL_SUB
```

Second call:

```
Substructures MSSQL
              RXN
              ecseSQLServer.dll
              <Server>
              <Database>
              LoginType=WINDOWS
              $$WINAUTH$$
              $$WINAUTH$$
              EC_LAB_RXN_BD
              EC_LAB_RXN_STR
              EC_LAB_RXN_SUB
```

In both calls you must provide the name of your SQL Server instance for "<Server>" and the name of your database for "<Database>"

## Creating Users

During the installation the operating system groups described in the table below are created on the ensochemLab web server. These groups are registered in SQL Server as logins with Windows authentication. For each of these logins an account is created in the database and the appropriate role is granted.

Operating system group / SQL Server login	SQL Server role
ensochemLab Database Readers	EC_LAB_READ
ensochemLab Database Writers	EC_LAB_REG
ensochemLab Database Admins	EC_LAB_ADMIN

With a manual installation you must perform all of these actions yourself. Doing this you can use different names and identifiers as long as the role names stay unchanged.

## 5. Creating Users

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During installation the following operating system groups have been created on your ensochemLab web server:

Read access:	ensochemLab Database Readers
Write access:	ensochemLab Database Writers
Administration:	ensochemLab Database Admins

Adding a user is very straightforward. Just use the administration tools of Windows to make him a member of one of these groups.

## 6. Configuration

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The database specific configuration is created by the setup program. Setup modifies the file "APP.config" and creates the two new files "Databases.mol" and "Databases.rxn".

Normally you must only define the two URLs for your virtual directory.

### **URL for ensochemEditor Web Edition**

If Setup runs on the server it tries to find out the two URLs and save them in the database. You should check the information in the administration dialog of ensochemLab client and make corrections if necessary.

### **URL for ensochemLab Webservice**

This URL must be entered in the client's configuration file as show in the following example (you must replace <SERVER> with the correct address):

```
[ensochemLab]
Service=http://<SERVER>/ensochemLab/ensochemLabService
```

The client setup program asks for this information and writes it to the client's configuration file.

# 7. Configuration Files

---

**Warning** The configuration files of ensochemLab server should never be modified manually. Any change can cause that the server stops working correctly. Be sure to make a backup of your configuration file before making any changes!

## Configuration File of ensochemLab Server

The folder "cfg" below the virtual directory of ensochemLab server contains the file "APP.config". When the file was initially copied from the CD it contains five entries, here marked in **blue** which must be changed.

```
<?xml version="1.0" encoding="utf-8" ?>
<configuration>

  <configSections>
    <sectionGroup name="databases">
      <sectionGroup name="default">
        <section name="general"
          type="enso.App.ecl.Server.NameValueSectionHandler,
            enso.App.ecl.Server.Config">
        </section>
        <section name="chemistry"
          type="enso.App.ecl.Server.NameValueSectionHandler,
            enso.App.ecl.Server.Config">
        </section>
        <section name="settings"
          type="enso.App.ecl.Server.NameValueSectionHandler,
            enso.App.ecl.Server.Config">
        </section>
        <section name="displayNames"
          type="enso.App.ecl.Server.NameValueSectionHandler,
            enso.App.ecl.Server.Config">
        </section>
      </sectionGroup>
    </sectionGroup>
  </configSections>

  <databases>
    <default>
      <general>
        <add key="DatabaseType" value="MSSQL"/>
        <add key="Server" value="$$SERVER$$"/>
        <add key="Database" value="$$DATABASE$$"/>
        <add key="Provider" value="SQLOLEDB.1"/>
        <add key="Parameters" value=""/>
        <add key="AutoLogin" value="$$AUTOLOGIN$$"/>
        <add key="ObjectPrefix" value="$$OBJPREF$$"/>
        <add key="ObjectSuffix" value=""/>
        <add key="InternalVersion" value="600"/>
      </general>
      <chemistry>
        <add key="Interface" value="Driver"/>
        <add key="ServerUrl" value="NOT USED"/>
        <add key="DriverRxn" value="ENSOCHEMLAB_RXN"/>
        <add key="DriverMol" value="ENSOCHEMLAB_MOL"/>
      </chemistry>
    </default>
  </databases>
</configuration>
```

```

        <add key="StereoChemistry" value="1"/>
        <add key="DatabaseType" value="$$CHEMDBTYPE$$"/>
    </chemistry>
    <settings>
        <add key="UseCatalog" value="1"/>
        <add key="ExternalUserData" value="0"/>
        <add key="CanEditExperimentNo" value="1"/>
        <add key="CanDeleteExperiment" value="1"/>
        <add key="CanOverwriteProjectList" value="1"/>
        <add key="CanOverwriteDepartmentList" value="1"/>
        <add key="CanOverwriteLaboratoryList" value="1"/>
        <add key="RemoveNoStructures" value="0"/>
        <add key="FuncGetNewExperimentNo" value="" />
        <add key="FuncGetNewTargetName" value="" />
        <add key="QueryBuilderConfig" value="QueryBuilder.config"/>

        <!-- one of the following entries, default is never
        <add key="InvalidateOnDelete" value="never"/>
        <add key="InvalidateOnDelete" value="always"/>
        <add key="InvalidateOnDelete" value="withRevisions"/>
        -->

        <!-- only possible when revisons plug-in is installed
        one of the following entries, default is never
        <add key="CreateNewRevision" value="never"/>
        <add key="CreateNewRevision" value="always"/>
        <add key="CreateNewRevision" value="finalized"/>
        <add key="CreateNewRevision" value="ownerChanged"/>
        <add key="CreateNewRevision" value="finalized, ownerChanged"/>
        -->

        <add key="CustomDataHandler" value="ecl"/>

    </settings>
    <displayNames>
        <add key="default" value="My General Database"/>
        <add key="DE" value="Standard Datenbank"/>
        <add key="EN" value="Default Database"/>
    </displayNames>
    </default>
</databases>

<appSettings>
    <add key="defaultDatabase" value="default"/>
    <add key="DefaultChemEditor" value="8"/>
    <add key="Print3Signatures" value="1"/>
    <add key="BinaryConverter" value="BinConverter"/>
    <add key="ConvertBinaryTo" value="PNG"/>
</appSettings>
</configuration>

```

Please replace the placeholders according to the table below

	Value
\$\$SERVER\$\$	The name of your SQL Server
\$\$DATABASE\$\$	The name of your database for alphanumerical data
\$\$AUTOLOGIN\$\$	Please enter the value "1".
\$\$OBJPREF\$\$	The schema of your alphanumerical database (i.e. "dbo.")
\$\$CHEMDBTYPE\$\$	Please enter the text "enso".

These changes are applied automatically when the installation is done with the setup program.

## Configuration Files of the Chemistry Database

Normally both configuration files for the chemistry database, "Databases.mol" and "Databases.rxn", will be created automatically by the setup program. For a manual installation you must create the files yourself and put them in the subdirectory "cfg" below the virtual directory of ensochemLab server

### Databases.mol

```
[ECDrvECS0102xx]

Type=MOL
Driver=ecseSQLServer.dll

Server=<SQL Server instance>
Database=<Chemistry database>
LoginType=WINDOWS
User=Dummy
Password=Dummy
BinData=EC_LAB_MOL_BD
StructData=EC_LAB_MOL_STR
Substructures=EC_LAB_MOL_SUB
```

### Databases.rxn

```
[ECDrvECS0102xx]

Type=RXN
Driver=ecseSQLServer.dll

Server=<SQL Server instance>
Database=<Chemistry database>
LoginType=WINDOWS
User=Dummy
Password=Dummy
BinData=EC_LAB_RXN_BD
StructData=EC_LAB_RXN_STR
Substructures=EC_LAB_RXN_SUB
```

Please replace in both file the values marked in **blue** with the correct information for your environment.

