



Installation guide V-NMR 1.5

This installation guide will help you to install version 1.5 of V-NMR on a server.

Requirements

- MySQL database server
- WEB server supporting PHP version 5.0.0 or higher with Mcrypt
- Access to an operational SMTP server

Installation

1. Unpack the downloaded archive "V-NMR".
2. Create a database on your server, create and/or configure a user account to manage it and import the database script found in root of the unpacked archive, "V-NMR.sql".
3. Create a (no-reply) e-mail address which the application may use to send e-mails through the SMTP server to (new/updated) configured users.
4. Open the file "databaseCommands.php" in the folder "V-NMR" and set the correct values underneath "//Variables to be changed when installed on a new server" at the top of the file. See below for an explanation of the different variables.
5. Place all content of the folder "V-NMR" within the desired folder of your WEB server.
6. Make sure the web server and database server are operational, open a browser and go to the webpage on which the application is installed.
7. Log in with the username "Admin" and the password "admin".
8. Go to "Staff" -> "Add / edit users" -> "Edit users" and select the user "Admin" to change the specific information to your personal information. To change the password you have to go to "Tools" -> "Change your password".
9. Optionally, go to "Staff" -> "Add / edit contact persons" -> "Add contact person" or "Edit contact person" and add or change the required information. (Contact persons (i.e. staff members) can be contacted by users via email through "Help" -> "E-mail staff".)

After those steps the application is installed. Now you can add molecules, solvents and samples to compute NMR spectra. For your convenience some sample monsters are added. You can add users, so that more people can make use of the application installed on your server. Please keep in mind that by default visitors have access to the application. This can be turned off in the "Add / edit users" menu.

PHP variables

The next list is an overview of the variables in the file "databaseCommands.php" that have to be set to install the application successfully. Not filling in those variables or filling in the wrong values may result in an not or incorrect working application.

- **\$crypto_connection:** This is the key that verifies (on a low level) whether or not it is the Flash application that wants to communicate with the PHP page. This key will only be changed with a new update of the application. Don't change it yourself.

- **\$crypto_key1:** Together with \$crypto_key2 this key is used to set the key for the encryption and decryption of the passwords which are placed into or read from the database. There are no length or character restrictions.
- **\$crypto_key2:** See \$crypto_key1.
- **\$crypto_key3:** Together with \$crypto_key4 this key is used to set the initialization vector for the encryption and decryption of the passwords which are placed into or read from the database. There are no length or character restrictions.
- **\$crypto_key4:** See \$crypto_key3.

- **\$db_host:** The name of the host where the database server operates on (*'localhost'* when it's the same computer as the web server).
- **\$db_name:** The name of the database.
- **\$db_username:** The name of the user that is configured to manage the database.
- **\$db_password:** The password of the managing user.

- **\$mail_host:** The name of the SMTP server that will be used to send emails.
- **\$mail_port:** The port number used by the SMTP server.
- **\$mail_authenticate:** Set to *'false'* if no authentication must be used when sending emails to the SMTP server, otherwise set to *'true'*.
- **\$mail_username:** The name of the user that will be used to authenticate with the SMTP server (this could be the no-reply e-mail address). Only used when *'\$mail_authenticate'* is set to *'true'*.
- **\$mail_password:** Password of the specified authentication user. Only used when *'\$mail_authenticate'* is set to *'true'*.
- **\$mail_from:** The no-reply e-mail address. This address is used when the V-NMR application must send emails to (new) users.

Installation problems, bug reports or improvement suggestions

When you access the V-NMR website for the first time you should see a login screen with a [Log-in] button and a [Visitor] button. You should be able to login. If this is not the case check your web server settings and/or your PHP settings. There is probably a wrong configuration setting.

Any bugs with or suggestions for VirtualNMR can be reported to support@VirtualNMR.org.

Help

For further information about using the V-NMR application see the online help from within the application or the website www.VirtualNMR.org.