

## **Installation and administrator guide for nmrshiftdb2:<sup>1</sup>** (Stand 05/05/17):

*This guide is will give you instructions for setup, installation and administration of nmrshiftdb2 on a local server. It contains information on operational concept and preconditions for setting up a server, and provides hands-on instructions for the installation. It is intended for administrators with system knowledge, specifically MySQL and Java application server knowledge is needed.*

*Revision history:*

See svn on [http://sourceforge.net/p/nmrshiftdb2/code/824/log/?path=/trunk/nmrshiftdb2/src/html/labhelp/install\\_nmrshiftdb2\\_en.docx](http://sourceforge.net/p/nmrshiftdb2/code/824/log/?path=/trunk/nmrshiftdb2/src/html/labhelp/install_nmrshiftdb2_en.docx)

and

<http://nmrshiftdb.svn.sourceforge.net/viewvc/nmrshiftdb/trunk/nmrshiftdb/doc/administratorguide.rtf?view=log>

*for the original NMRShiftDB document*

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*nmrshiftdb2* is developed by Stefan Kuhn and the NMR facility at University of Cologne. The precursor, NMRshiftDB, was the developed by the Steinbeck lab (EBI Cambridge). Further informations are available on the general homepage, <http://www.nmrshiftdb.org/>.

## 1. Operational concept of nmrshiftdb2

**nmrshiftdb2** is a J2EE web application based on the Jetspeed framework for portals. This means, it is an application running in an application server and is used via a browser. Instances can run independently from other nmrshiftdb2 instances, i.e. you can use, but are not obliged to, existing data from the sf.net download page (<http://sourceforge.net/projects/nmrshiftdb2/files/nmrshiftdb2/>).

## 2. Installation of nmrshiftdb2 (local server)

The installation of the software requires to install some prerequisites (e. g. the database server) and the deployment of a war file to tomcat. This war file must have some changes of configuration files to the required values. There are three possible ways to get such a war file:

- Download a binary pre-compiled war file from <https://sourceforge.net/projects/nmrshiftdb2/files/> and change this. This requires unpacking and re-packing the file and is not recommended.
- Checkout the source code from the subversion repository by the `svn co svn://svn.code.sf.net/p/nmrshiftdb2/code/trunk/nmrshiftdb2 nmrshiftdb2` command. This will give you the current version, which may not be as stable as desired.
- We recommend to download the latest source version from <https://sourceforge.net/projects/nmrshiftdb2/files/>

The following chapter describes prerequisites and step-by-step installation if you want to setup **nmrshiftdb2** on your local server. We use CentOS for our servers. Other operating systems and Linux version should work, but are not tested. You need to modify the steps as required.

### 2.1 Prerequisites

All of the following software packages are needed and should be installed via the package manager (yum on CentOS).

- Ant (1.6 or higher)
- Java Development Kit (version 1.7 or higher is needed). On CentOS OpenJDK is provided, which works as well as the Sun JDK
- MySQL database server (version 5.0 or later is needed). On CentOS the „mysql-server“ package provides this. Package „mysql“ contains the client, which is needed for maintenance. The use of other database systems would require changes, e. g. to the UDFs (see 2.2 (6)) and probably also to the sql in the Java code.
- Apache web server (if you want to run tomcat as an apache module, which is recommended). On CentOS, the package is called httpd.
- Apache axis2 (use version 1.7.4). This is available from [http://www.apache.org/dyn/closer.cgi/ws/axis/1\\_4](http://www.apache.org/dyn/closer.cgi/ws/axis/1_4). This is only needed if you want to run the web services.
- Tomcat (the latest version of the 5, 6, and 7 branches work). On CentOS the package is called „tomcatX“ where X is 5, 6, or 7.
- With respect to hardware any current server system should do. 2 GB of RAM are recommended. For checkout and installation of the nmrshiftdb2 software 4 GB should be available. The

database size depends on the content. For guidance, the public database at the end of 2014 was 3 GB.

## 2.2 Installation: Step-by-step instructions

(1) If you have downloaded and unpacked the source release or checked out the source code from the SVN you have got a new directory "nmrshiftdb2" with subdirectories.

(2) If you want to run MySQL on the same server as tomcat does, no changes are necessary. This is likely to be the default. Otherwise, you need to tell nmrshiftdb2 where the database server is running: In the file nmrshiftdb2/src/conf/jetspeed/WEB-INF/conf/Torque.properties there is a line

```
torque.database.nmrshiftdb.url = jdbc:mysql://127.0.0.1/nmrshiftdb
```

You need to change these settings for your database. If you wanted to use a database system other than MySQL, you have to change the lines around here as well (you will then probably need to change the sql scripts (see (4) as well). Please note, that this has not been tested. **In order to participate in the nmrshiftdb2 network you need to use MySQL anyway, because this relies on the MySQL replication mechanism.**

(3) In order to have unicode working, the following lines must be in my.cnf file:

```
[mysqld]  
character-set-server = utf8  
collation-server = utf8_unicode_ci
```

Check other mysql settings as needed in your setup.

(4) Make sure the mysql header files are installed. On Linux, a package called mysql-devel might be needed, depending on the distribution. As a fallback solution you can also copy all .h-files from nmrshiftdb2/src/c++ to the include-directory for shared libraries, which is usually /usr/include on Linux systems, but the headers for your distribution are better, since they match the version.

(5) Compile the file nmrshiftdb2/src/c++/udf\_nmrshiftdb.cc with command line command:

```
'g++ -shared -fPIC -o udf_nmrshiftdb.so udf_nmrshiftdb.cc'
```

to the directory for shared libraries, which is usually /usr/lib/ on Linux systems.

(6) Compile the file nmrshiftdb2/src/c++/spectrumsimilarity.cc with:

```
'g++ -shared -fPIC -o spectrumsimilarity.so spectrumsimilarity.cc'
```

to the directory for shared libraries, usually /usr/lib/ on Linux-Systems.

(7) Create an empty database "nmrshiftdb". This is done by typing

```
create database nmrshiftdb;
```

in the mysql command line client. Please, refer to the documentation on <http://www.mysql.org> to learn how to setup, use and administer MySQL.

(8) Make sure unicode is used for your new database. You can change this with the MySQL command `ALTER DATABASE nmrshiftdb CHARACTER SET utf8`; if necessary.

(9) Change the passwords in `nmrshiftdb2/src/sql/populate-mysql.sql`, especially for the admin user. The passwords are the fifth value in the lines starting with `INSERT INTO TURBINE_USER`. By default, the admin password is "admin", for example.

(10) In order to have Unicode used in MySQL, use the MySQL command `SET NAMES utf8` (from mysql 5.5.3, `utf8mb4` might also be a choice, supporting more characters). This might not be necessary on new MySQL installations. Check the manual if in doubt.

(11) In `nmrshiftdb2/src/sql` there are five sql scripts you need to run (`security-schema.sql`, `dbpsml-schema.sql`, `nmrshiftdb-schema.sql`, `id-table-schema.sql`, `populate-mysql.sql`). This is done by issuing the command line commands

```
mysql -u root -p nmrshiftdb < dbpsml.sql
```

for this and (likewise) for the other sql files from the command line. If you have a mysql version <5.5 (or your default table type is not InnoDB for some reason) then you also need to run `innodb-pre-5.5.sql` (this changes table types to InnoDB and creates foreign keys). **If you want to use the lab system (LIMS), also run `populate-labsystem.sql`.**

(12) You need to grant access to the `nmrshiftdb2` database to the user specified in `./src/conf/jetspeed/WEB-INF/conf/Torque.properties`. You'll see the lines

```
torque.dsfactory.default.connection.driver=  
com.mysql.jdbc.Driver  
torque.dsfactory.default.connection.url=  
jdbc:mysql://localhost:3306/nmrshiftdb?autoReconnect=true  
torque.dsfactory.default.connection.user=  
nmrshiftdbuser  
torque.dsfactory.default.connection.password=  
nmrshiftdbuser
```

In order to create the user "nmrshiftdbuser", issue the MySQL command

```
CREATE USER nmrshiftdbuser [IDENTIFIED BY 'nmrshiftdbuser']
```

Of course, you can use a better password here, but make sure to put it into `Torque.properties`. Log into mysql (`mysql -u root -p`) and issue the MySQL command

```
GRANT ALL PRIVILEGES ON nmrshiftdb.* TO 'nmrshiftdbuser'@'localhost'  
IDENTIFIED BY 'nmrshiftdbuser' WITH GRANT OPTION;
```

(13) Change the Tomcat path in `nmrshiftdb/2build.properties` to the appropriate value. This path must point to the directory in your tomcat installation containing the `servlet-api.jar`. This is `/var/lib/tomcat5/common/lib/` on CentOS.

(14) We use jni-inchi for generating inchis. In order to get this working I found it was necessary to do:

```
mkdir /usr/share/tomcatX/.jnati
```

and

```
chown tomcat:tomcat /usr/share/tomcatX/.jnati
```

This has to do with rights of the user under which tomcat runs to create a directory for the inchi libraries. Exact locations and user name probably depends on installation and tomcat version.

(15) If you want to install the web services follow section 3 after you installed nmrshiftdb2. In nmrshiftdb2 you need to remove the jars jnati-core-0.4.jar, jnati-deploy-0.4.jar, log4j-1.2.15.jar and jni-inchi-0.8.jar from the lib directory and put them into /var/lib/tomcatX/common/lib/ or the respective directory of your tomcat installation. If the web services are not needed you do not need to do anything here.

(16) The file src/vmtemplates/news.html will be part of the home page, you can put any content you like (the news on [www.nmrshiftdb.org](http://www.nmrshiftdb.org) are fetched from sf.net by a cron job).

(17) If your application does not run in the root context (see 21), you need to change src/java/org/openscience/nmrshiftdb/util/UrlTool.java. The line

```
url.append(st.nextToken()+"/portal");
```

must become

```
url.append(st.nextToken()+"/<your_context_name>/portal");
```

(18) Have a look at the nmrshiftdb2/src/conf/jetspeed/WEB-INF/conf/NMRShiftDB.properties file. Entries are explained in the file. Set them as needed. There is a separate chapter below on the choice of editor. Also have a look at nmrshiftdb2/src/conf/jetspeed/WEB-INF/conf/log4j.properties – default location for log files is the tomcat logs dir.

(19) Add the following lines to your apache configuration:

```
RewriteEngine on
RewriteRule ^/molecule/([0-9]*)$ /portal/js_pane/P-
Results/nmrshiftdbaction/showDetailsFromHome/molNumber/$1 [R]
RewriteRule ^/molecule/([0-9]*)/dataset/(.*)$ /portal/js_pane/P-
Results/nmrshiftdbaction/showDetailsFromHome/molNumber/$1/dataset/
$2 [R]
RewriteRule ^/molecule/([0-9]*)/dataset/(.*)$ /portal/js_pane/P-
Results/nmrshiftdbaction/showDetailsFromHome/molNumber/$1/dataset/
$2 [R]
RewriteRule ^/atom/([0-9]*)$ /portal/js_pane/P-
Results/nmrshiftdbaction/showDetailsFromHome/molNumber/atom:$1 [R]
```

```
RewriteRule ^/spectrum/([0-9]*)$ /portal/js_pane/P-  
Results/nmrshiftdbaction/generalsearch/searchfield/spectrum+id/sear  
chaction/exact/searchstring/$1#spectrum$1 [NE,L,R]
```

This will make short URLs possible. If you do not use mod\_jk, this is not possible. For the main nmrshiftdb2 server, mod\_jk should always be used and the redirection be installed.

(20) Running the `ant dist` command on command line in the `nmrshiftdb2` directory (the SVN checkout) will create a `jetspeed.war` in the `nmrshiftdb2/dist` directory.

(21) Copy that file to `$TOMCAT_HOME/webapps/`. The name of the file will be the context in which your application runs. If you call it `ROOT.war`, the application will run in the root context, i. e. it can be called with an URL like `http://servername/`, else it will be like `http://servername/jetspeed`. See Tomcat manuals if you are not sure.

(22) Start tomcat with `$TOMCAT_HOME/bin/startup.sh`

(23) Go to the URL `http://yourmachine:8080/index.jsp`. If you have tomcat running as an apache module, it will be available via the apache port, normally 80. You can then close the 8080 port on tomcat. If you want to run tomcat as an apache module, using mod\_jk, Apache must be instructed to serve some files from tomcat. The entry in the `httpd.conf` file should look like this:

```
JkMount /nmrshiftdb wlb  
JkMount /nmrshiftdb/* wlb  
JkMount  
/portal wlb  
JkMount /portal/* wlb  
JkMount /NmrshiftdbServlet wlb  
JkMount /NmrshiftdbServlet/* wlb  
JkMount /download/* wlb  
JkMount /*.jsp wlb  
JkMount /axis2 wlb  
JkMount /axis2/* wlb  
JkMount /*.captcha wlb
```

(24) If you see the nmrshiftdb homepage, the installation did work. Try to login as one of the users from `populate-mysql.sql`.

(25) If you checkout `svn://svn.code.sf.net/p/nmrshiftdb2/code/trunk/nmrshiftdb2-webservices` you can run tests for your installation. This is highly recommended. Update the server url in `TestConstants.java` and run the `TestSuite` class

(26) If you want to run the lab system, continue with the lab system admin guide at <http://sourceforge.net/p/nmrshiftdb2/wiki/LabSystemAdmin/>. Notice that the `populate-labsystem` script created user `nmruser` (configured as the lab admin), `testworker` (a lab coworker/staff member) and `testuser` (a user) with their usernames as passwords by default.

### 3. Structure editors in nmrshiftdb2

You have a choice of structure editors to use in nmrshiftdb2. Which one is used is set in the NMRShiftDB.properties file. Currently the following options exist:

- JCP: The JChemPaint applet. This is a fully functional, rich Java Applet. It works well, but usage is problematic, since support for JChemPaint seems to have stopped and the Java Applet technology in general has not had a good name recently.
- MARVINJS: This is the Marvin JS application by Chemaxon. The code is contained in the checkout, but you need a license to operate this. Licenses are available from Chemaxon, in some cases also for free. Check with Chemaxon for your requirements. In order to get all functions of Marvin JS, you need to install the JChem Webservices in your tomcat. See <http://www.chemaxon.com/download/jchem-suite/>

#### 4. Installation of the web services

Prerequisites are as for the nmrshiftdb2 project itself. The webservices must be installed alongside the nmrshiftdb2 application in one tomcat instance. You need to download the src package or checkout the code from `svn://svn.code.sf.net/p/nmrshiftdb2/code/trunk/nmrshiftdb2-webservices`

- (1) If you have downloaded and unpacked the source release or checked out the source code from the SVN you have got a new directory "nmrshiftdb2-webservices" with subdirectories.
- (2) Make the environment variable `AXIS2_HOME` point to the nmrshiftdb2-webservices directory (this works, if you have the full axis2 downloaded, you can use that as well). Run `ant jar.server` in this directory.
- (3) Download axis2 from <http://axis.apache.org/axis2/java/core/download.cgi>. Version 1.7.4 has been tested. It should be enough to get the binary distribution. Deploy the war file to your tomcat.
- (4) Copy the jars from the lib directory of the nmrshiftdb2-webservices project into the `WEB-INF/lib` directory of the expanded war file. Also copy the following jars from the lib directory of the nmrshiftdb2 project (notice that copying all will cause version conflicts): `activemq-1.0.jar`, `aopalliance-1.0.jar`, `avalon-framework-api-4.3.1.jar`, `avalon-framework-impl-4.3.1.jar`, `batik-all-1.8.jar`, `beam-core-0.9.2.jar`, `beam-func-0.9.2.jar`, `bsws-1.0.jar`, `cage-1.0.jar`, `castor-0.9.3.jar`, `cdk-*.jar`, `cglib-full-2.0.2.jar`, `cmlxom-2.5-b1.jar`, `commons-beanutils-1.6.1.jar`, `commons-collections-3.0.jar`, `commons-configuration-1.0-dev.jar`, `commons-dbc-1.2.1.jar`, `commons-digester-1.7.jar`, `commons-discovery-0.2.jar`, `commons-lang-2.0.jar`, `commons-pool-1.2.jar`, `concurrent-1.3.4.jar`, `cos.jar`, `ecs-1.4.1.jar`, `fontbox-1.8.5.jar`, `fop.jar`, `fulcrum-3.0-b2-dev.jar`, `graph.jar`, `guava-17.0.jar`, `iText-2.1.7.jar`, `itext-asian.jar`, `jasperreports-4.1.1.jar`, `jaxrpc-1.1.jar`, `JCampParser.jar`, `jcs-1.0-dev.jar`, `jetspeed.jar`, `jgrapht.jar`, `JNL.jar`, `jsch-0.1.53.jar`, `jzlib-1.1.1.jar`, `libsvm.jar`, `mysql-connector-java-5.1.28-bin.jar`, `nmrshiftdb.jar`, `nmrshiftdb-lib.jar`, `oro-2.0.7.jar`, `regex-1.2.jar`, `saaj-1.1.jar`, `serializer-2.7.0.jar`, `slf4j-api-1.7.12.jar`, `slf4j-simple-1.7.12.jar`, `soap-2.1.jar`, `spectrumapplet.jar`, `spring-1.1.5.jar`, `sshj-0.8.1.jar`, `stratum-1.0-b4-dev.jar`, `torque-3.1.jar`, `turbine-2.2.jar`, `uddi4j-1.0.jar`, `vecmath1.2-1.14.jar`, `velocity-1.4.jar`, `village-1.5.3-dev.jar`, `weka.jar`
- (5) Copy the file `build/lib/NMRShiftDB.aar` into the `WEB-INF/services/` directory of your tomcat installation. The services should be installed automatically. Go to <http://nmr-sdbtest.nmr.uni-koeln.de/axis2/services/listServices> to check that the nmrshiftdb2 web services are listed.