

# //////////////////////////////////// INSTALLATION ////////////////////////////////////

#

## # Requirements

#

```
[me@mach ~]$ uname -a
Linux mach 2.6.18-238.19.1.el5PAE #1 SMP Fri Jul 15 08:15:44 EDT 2011 i686 athlon i386
GNU/Linux
```

```
[me@mach ~]$ cat /etc/redhat-release
CentOS release 5.6 (Final)
```

```
[me@mach ~]$ which gnuplot
/usr/local/bin/gnuplot
```

```
[me@mach ~]$ /usr/local/bin/gnuplot -V
gnuplot 4.3 patchlevel 0
```

```
[me@mach ~]$ /usr/sbin/httpd -v
Server version: Apache/2.2.3
Server built:   May  4 2011 06:51:15
```

```
[me@mach ~]$ /usr/sbin/httpd -l
Compiled in modules:
  core.c
  prefork.c
  http_core.c
  mod_so.c
```

```
[me@mach ~]$ php -v
PHP 5.1.6 (cli) (built: Nov 29 2010 16:47:37)
Copyright (c) 1997-2006 The PHP Group
Zend Engine v2.1.0, Copyright (c) 1998-2006 Zend Technologies
```

#

## # uncompress the nmrview.tar.gz archive

#

```
[me@mach softs]$ pwd
/opt/softs
```

```
[me@mach softs]$ ll ./nmrview.tar.gz
-rw-r--r-- 1 me users 20401644 Mar 26 15:44 ./nmrview.tar.gz
```

```
[me@mach softs]$ tar xvzf ./nmrview.tar.gz
./nmrview/
./nmrview/www/
./nmrview/www/tmp
./nmrview/www/js/
./nmrview/www/js/spectrum.js
./nmrview/www/js/ui.nmrview.js
./nmrview/www/js/utills.js
./nmrview/www/etc
./nmrview/www/images/
./nmrview/www/images/img_00.gif
./nmrview/www/images/loading.gif
./nmrview/www/inc/
./nmrview/www/inc/Set_Config.inc
./nmrview/www/inc/config.inc
./nmrview/www/inc/getnmrspec.inc
```

```

./nmrview/www/inc/main.inc
./nmrview/www/inc/nmrproc_conf.inc
./nmrview/www/inc/nmrproc_ui.inc
./nmrview/www/inc/nmrproc_view.inc
./nmrview/www/.htaccess
./nmrview/www/css/
./nmrview/www/css/redmond/
./nmrview/www/css/redmond/images/
./nmrview/www/css/redmond/images/ui-icons_217bc0_256x240.png
./nmrview/www/css/redmond/images/animated-overlay.gif
./nmrview/www/css/redmond/images/ui-bg_gloss-wave_55_5c9ccc_500x100.png
./nmrview/www/css/redmond/images/ui-bg_flat_0_aaaaaa_40x100.png
./nmrview/www/css/redmond/images/ui-bg_flat_55_fbec88_40x100.png
./nmrview/www/css/redmond/images/ui-bg_glass_75_d0e5f5_1x400.png
./nmrview/www/css/redmond/images/ui-bg_glass_85_dfeffc_1x400.png
./nmrview/www/css/redmond/images/ui-bg_glass_95_fef1ec_1x400.png
./nmrview/www/css/redmond/images/ui-bg_inset-hard_100_f5f8f9_1x100.png
./nmrview/www/css/redmond/images/ui-bg_inset-hard_100_fcfdfd_1x100.png
./nmrview/www/css/redmond/images/ui-icons_2e83ff_256x240.png
./nmrview/www/css/redmond/images/ui-icons_469bdd_256x240.png
./nmrview/www/css/redmond/images/ui-icons_6da8d5_256x240.png
./nmrview/www/css/redmond/images/ui-icons_cd0a0a_256x240.png
./nmrview/www/css/redmond/images/ui-icons_d8e7f3_256x240.png
./nmrview/www/css/redmond/images/ui-icons_f9bd01_256x240.png
./nmrview/www/css/redmond/jquery-ui.min.css
./nmrview/www/css/redmond/jquery-ui.css
./nmrview/www/css/redmond/jquery.ui.theme.css
./nmrview/www/view
./nmrview/www/log/
./nmrview/www/log/tracing/
./nmrview/www/view.php
./nmrview/etc/
./nmrview/etc/nmrproc.conf
./nmrview/bin/
./nmrview/bin/corrige_lr
./nmrview/bin/pack_lr
./nmrview/bin/bin4gp_lr
./nmrview/bin/geoloc_check
./nmrview/bin/pack Bruker
./nmrview/bin/pack_jdx
./nmrview/bin/parserBruker
./nmrview/bin/parserJCAMP
./nmrview/bin/parserJCAMP.pl
./nmrview/bin/tab2csv
./nmrview/examples/
./nmrview/examples/simple.html
./nmrview/tmp/

```

```
[me@mach projets]$ cd nmrview
```

```

[me@mach nmrview]$ ll
total 24
drwxr-xr-x 2 me users 4096 Mar 26 15:13 bin
drwxr-xr-x 2 me users 4096 Mar 26 15:16 etc
drwxr-xr-x 2 me users 4096 Mar 26 15:29 examples
drwxr-xr-x 2 me users 4096 Mar 26 15:29 tmp
drwxr-xr-x 7 me users 4096 Mar 26 15:27 www

```

#

# gives the right permissions for apache

#

```
[me@mach nmrview]$ chmod 777 tmp
```

```
[me@mach nmrview]$ chmod -R 777 ./www/log/
```

#

## # Edit the configuration files

#

```
[me@mach nmrview]$ vi ./etc/nmrproc.conf
```

```
-----  
# Warning: Take care not putting spaces each side of equal sign, in order to be executed as a  
script shell
```

```
# VARNAME=anything including spaces
```

```
# The root of the bulk of your installation.
```

```
# Think to create a symbolic link under the HTML document directory of your web server which  
points to the www directory of nmrview.
```

```
ROOTDIR=/opt/softs/nmrview
```

```
# The root of the datasets
```

```
DATASETS=/opt/data/nmrview
```

```
# The root of the URL
```

```
URLROOT=/nmrview
```

```
# default NMR spectrum parameters
```

```
SOLVENT_MIN=4.7
```

```
SOLVENT_MAX=4.97
```

```
PPM_MIN=-0.05
```

```
PPM_MAX=11
```

```
...
```

#

**# Create a symbolic link under the HTML document directory of your web server**

**# which points to the www directory of nmrview.**

#

```
[me@mach nmrview]$ cd /var/www/html/
```

```
[me@mach nmrview]$ sudo ln -s /opt/softs/nmrview/www nmrview
```

////////////////////////////////////

**How to process with an ISA-TAB archive?**

////////////////////////////////////

#

**# unzip the isatab archive in a temporary directory**

#

```
[me@mach ~]$ unzip HUGO07.isa -d /tmp/HUGO07/
```

```
Archive:  HUGO07.isa
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13091.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13092.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13101.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13102.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13111.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13112.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13121.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13122.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13131.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13132.zip
```

```
  extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13141.zip
```

```

extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13142.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13151.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13152.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13161.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13162.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13171.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13172.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13181.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13182.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13191.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13192.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13201.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13202.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13331.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13332.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13341.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13342.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13351.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13352.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13361.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13362.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13371.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13372.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13381.zip
extracting: /tmp/HUGO07/BB_BBI_08M07_melon07_13382.zip
inflating: /tmp/HUGO07/a_hugo_2007_metabolite_profiling_NMR_spectroscopy.txt
inflating: /tmp/HUGO07/i_Investigation.txt
inflating: /tmp/HUGO07/s_Hugo_2007.txt

```

#

**# Convert isa\_tab metadata files into a CSV file**

#

```
[me@mach ~]$ cd /opt/softs/nmrview
```

```

[me@mach nmrview]$ ./bin/tab2csv -d /tmp/HUGO07/ -o samples.csv -v
i_Investigation.txt ... OK
s_Hugo_2007.txt ... OK
a_hugo_2007_metabolite_profiling_NMR_spectroscopy.txt ... OK
Extract columns from Study Assay File : 1,28 ...OK
Factors: ;Harvest date
Extract columns from Study File : 9,10 ... OK
Merging ...OK

```

#

**# Create an entry under the root of the datasets (see ./etc/nmrproc.conf)**

#

```
[me@mach nmrview]$ mkdir /opt/data/nmrview/HUGO07
```

#

**# Create the "pack" file : 'pack\_bruker' script is for bruker raw files**

#

```

[me@mach nmrview]$ time ./bin/pack_bruker -i /tmp/HUGO07/samples.csv \
-o /opt/data/nmrview/HUGO07/ -h

```

```

-----
BB_BBI_08M07_melon07_13091 (1/36) ...
NAME = 07.HU1.1.1309.1
OK

```

```

-----
BB_BBI_08M07_melon07_13092 (2/36) ...
NAME = 07.HU1.1.1309.2

```

```

OK
-----
BB_BBI_08M07_melon07_13101 (3/36) ...
NAME = 07.HU1.2.1310.1
OK
-----
BB_BBI_08M07_melon07_13102 (4/36) ...
NAME = 07.HU1.2.1310.2
OK
...

-----
BB_BBI_08M07_melon07_13372 (34/36) ...
NAME = 07.HU3.5.1337.2
OK
-----
BB_BBI_08M07_melon07_13381 (35/36) ...
NAME = 07.HU3.6.1338.1
OK
-----
BB_BBI_08M07_melon07_13382 (36/36) ...
NAME = 07.HU3.6.1338.2
OK
Pack ...OK

```

```

real    0m39.698s
user    0m13.305s
sys     0m9.039s

```

```

#
# Check if all files have been created

```

```

#
[me@mach nmrview]$ ll ./data/HUGO07/
total 9756
-rw-r--r-- 1 me users      28 Mar 27 17:57 factors
lrwxrwxrwx 1 me users      11 Mar 27 17:57 rawfile -> samples.csv
-rw-r--r-- 1 me users    1812 Mar 27 17:57 samples.csv
-rw-r--r-- 1 me users 9961496 Mar 27 17:58 specs.pack

```

```

#
# Create a simple html page using the example
#

```

```

[me@mach nmrview]$ cp examples/simple.html ./www/

[me@mach nmrview]$ vi ./www/simple.html
-----
change the line 13:
      url:'/nmrview/view',  dataset: 'exemple', colorby: 0, width: 'auto'
replace 'exemple' by 'HUGO07':
      url:'/nmrview/view',  dataset: 'HUGO7', colorby: 0, width: 'auto'
-----

```

```

#
# In your web browser, open the URL: http:<your domain>/nmrview/simple.html
#

```