

Mora the Explorer

Mora the Explorer is a small program that downloads your Bruker (up to 400 MHz) **and** your Agilent (500 & 600 MHz) NMR data directly onto your own computer. To use it, you need only to enter your acronym, your group and your destination folder. These options could be saved as defaults. For a current download, select between measurements up to 400 and measurements at 500 & 600 MHz and enter the day of the measurement. If something is found, it will be copied to your predefined target folder (e.g. I:\nmr)!

Mora the Explorer is © 2023 **Matthew J. Milner** and distributed open-source under the terms of the GNU General Public License version 3. The source code is available from the mora server at <mora>/nmr/mnova/mora_the_explorer/src/

1) Installation

Windows

- Create a destination folder for your spectra: e.g. **I:\nmr** (alternatively a local folder or a folder on your group disk)
- File explorer ⇒ Computer ⇒ map
 - drive : Z
 - folder : \\mora\nmr
 - connect as : NWZ\< your account >
- Download mora_the_explorer.zip from \nmr\mnova\mora_the_explorer\windows
- Click with right mouse button on the zip-file and extract it to wherever you want to install the program e.g. C:\Users\<your account>\
- Open the mora_the_explorer folder and find **mora_the_explorer.exe** within. This is the program.
- Optionally, to make the program easier to find in future, create a shortcut to mora_the_explorer.exe, or after starting the program for the first time, select the icon on the taskbar and choose “Pin to taskbar” or “An Taskleiste anheften”

macOS (11.7.9 or higher)

- Create a destination folder for your spectra: e.g. **/Users/klaube/nmr**
- Open finder ⇒ cmd-key K ⇒ smb://nwz;< your account >@mora.uni-muenster.de/nmr
- Download mora_the_explorer.app from nmr/mnova/mora_the_explorer/mac
- Move it to the Applications folder (“/Applications”, or “/Programme” on German Macs). This will make it show up in the Launchpad.

Linux

- Create a destination folder for your spectra: e.g. **~/nmr**
- Make sure the mora server is mounted with the appropriate permissions (see <https://www.uni-muenster.de/Chemie.oc/en/nmr/nmr-service.html> “Download of chemical data”)
- Download mora_the_explorer.tar.gz from <mora>/nmr/mnova/mora_the_explorer/linux and extract it to the desired location (e.g. ~/mora_the_explorer).
- The binary, called simply “mora_the_explorer”, can be found within the extracted directory.

2) Getting started

- Open the program according to your operating system as detailed above.
- Enter your personal details (1 and 2 in image)
- Type in or copy and paste the path of the folder you want your NMR spectra to be saved to.
- The **go to** button can be used to quickly open the folder you have given, but only after you’ve provided the path. It **doesn’t** let you choose the save location.
- Choose your settings for the formatting of the names of the saved folders (4 in image). By default, the spectra folders will be saved with names formatted as: 357-1-proton. With all

options selected, the spectra folders would be formatted so: `ams-357-1-proton-cdcl3`. The solvent cannot be included for Agilent 500/600 MHz spectra, however.

- f) Choose which spectrometer you would like to check (5 in image).
- g) For the routine, low-field Bruker spectrometers there is the option to check at a regular interval (6 in image). After pressing start, this will cause the program to repeatedly check for new spectra after the time specified has elapsed. This is somewhat unnecessary but some users may prefer it. Note that this option is not available on the Agilent high-field spectrometers.
- h) Save all the settings you just chose by clicking on the save button (7 in image)
- i) Finally, select the date on which the sample was **queued** for measurement (note that samples placed on a spectrometer on, for example, Monday evening but measured Tuesday morning are considered as belonging to Monday!). Pressing the **today** button will set the day to today's date. The option exists to search all dates **since** a given date, but this is designed to allow you to do a one-off check every now and again to make sure you did not forget to download any spectra – it should not be used on a regular basis!

Note that when searching the high-field spectrometer only the year must be provided, which will be checked in full, so the exact date of submission is unimportant. The other options described are thus not available when the high-field spectrometer is selected.

- j) Press **start check now** to perform a check with the given settings. The server will be checked for any spectra that **aren't already saved in the destination folder** with the same name. Multiple spectra with the same name (e.g. a day and night proton measurement of `ams-357-1`) will be numbered consecutively (e.g. `ams-357-1-proton` and `ams-357-proton-2`). Any spectra found will be listed in the box below, and a green banner will appear to let you know that new spectra were found, which can be dismissed with a click.

- ← 1. Enter your acronym
- ← 2. Choose your group
- ← 3. Enter your destination folder
- ← 4. Decide to include additional infos in filename
- ← 5. Choose either Bruker (up to 400 MHz) or Agilent data
- ← 6. Choose *repeat* or *single* check
- ← 7. Save as default
- ← 8. Choose the date, when the nmr measurement was saved
- ← 9. Start download

Local destination folder I:\nmr:

(I:) klaube (\\nwz.wvu.de\dfs\home\k) > nmr

Name

ges_540_neo400a_Aug15-2023_20-proton-CDCl3
ges_540_neo400a_Aug15-2023_21-carbon-CDCl3