

NMRFetch

Quick user guide

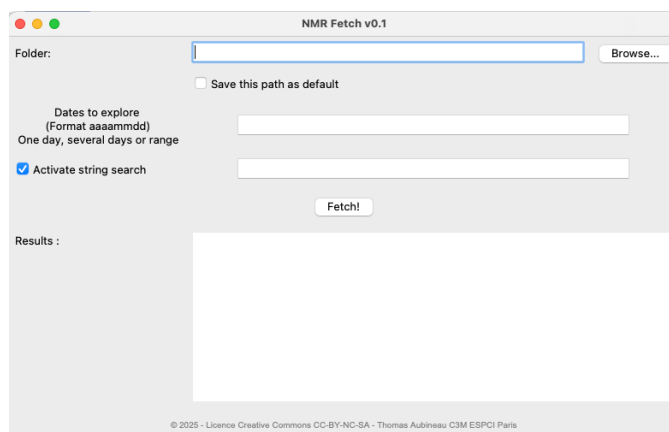
NMRFetch is a home/lab-made tool to facilitate the retrieving of NMR data in the Bruker root tree. It is based on Python script but does not need any python installed on the user's computer.

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App files may be downloaded from <https://github.com/taubineau/NMRFetch>

The Windows version is the .exe ; the MacOS version is in the .zip file.

Upon launching NMRFetch app, a window will open as shown below (MacOS version displayed but PC version is similar):



- Folder: Locate the main NMR folder where the data is archived. If the default folder is not the right one, click the “Browse” button or write the folder path. The root folder to start the search should always be the one containing the date folders and should look like <[User]/nmr> in standard Bruker root tree.

Example for MacOS: /Volumes/Data/data/CDM/nmr

Example for Windows: Y:/Data/data/CMC/nmr (where Y: is the letter assigned to the NMR network drive in Windows Explorer)

- You may tick the box to save the path as default for the next time.
- Dates: Chose which date folder(s) to explore, in aaaammdd format. To search one folder, input one date (*eg* 20250207). To search several folders, input them all separated by spaces (*eg* 20250103 20250205 20250207). To search all the folders in a range, input the range with a ‘-’ separator (*eg* 20250103-20250207)

- By default, the “Activate string search” is activated. Input the title of the experiment you are looking for. The search is not case sensitive and should not take the spaces into account (TA425 should give the same result as TA 425 and ta425). You may look for all or only a part of the sample title. If the box is unticked or the field left blank, the script will list all the experiments of the folder(s) as the result.

Click “*Fetch!*” to start the script.

- Results: The list of found corresponding titles is displayed with the following template

<EXPNO>/<PROCNO> : “*title*” (*exp*) as defined in Bruker nomenclature.

EXPNO is the date, PROCNO the processing number and *exp* the experiment actually performed (*eg* pro, 19F, C_CPD etc)

The results are sorted by increasing EXPNO and then increasing PROCNO

Examples:

The image displays two side-by-side screenshots of the 'NMR Fetch v0.1' application window. Both windows show the 'Folder:' field set to '/Volumes/Data/data/CDM/nmr' and the 'Dates to explore' field. The left window has '20250402' in the date field and 'Activate string search' checked. The right window has '20250329-20250402' in the date field and 'BW' in the search field. Both windows show a 'Fetch!' button and a 'Results:' section displaying a list of experiment titles in a specific format.

Left Screenshot Results:

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20250402/10 : "Utilisateur COM BLB EXT 30%" (pro)
20250402/11 : "Utilisateur COM test" (pro)
20250402/20 : "Utilisateur COM SL184 J+5" (pro)
20250402/30 : "Utilisateur COM SL85 M+" (pro)
20250402/40 : "Utilisateur COM AD-252-dried-total-CD2C12" (pro)
20250402/50 : "Utilisateur COM AD-252-dried-total-CD2C12" (C_CPD)
20250402/51 : "Utilisateur COM AD-252-dried-total-CD2C12" (C_DEPT135)
20250402/52 : "Utilisateur COM AD-252-dried-total-CD2C12" (pro)
20250402/53 : "Utilisateur COM AD-252-dried-total-CD2C12" (H_COSYGP5W)
20250402/54 : "Utilisateur COM AD-252-dried-total-CD2C12" (CH_HSQC6P)

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Right Screenshot Results:

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20250331/100 : "Utilisateur CMC BW944-F1" (pro)
20250331/181 : "Utilisateur CMC BW944-F1" (19F_CPD)
20250331/210 : "Utilisateur CMC BW944-F2" (pro)
20250331/250 : "Utilisateur CMC BW944-F1" (pro)
20250331/251 : "Utilisateur CMC BW944-F1" (C_DEPT135)
20250331/252 : "Utilisateur CMC BW944-F1" (pro)
20250331/253 : "Utilisateur CMC BW944-F1" (H_COSYGP5W)
20250331/254 : "Utilisateur CMC BW944-F1" (CH_HSQC6P)
20250401/20 : "Utilisateur CMC BW950-F2" (pro)
20250401/21 : "Utilisateur CMC BW950-F2" (19F_CPD)
20250402/40 : "Utilisateur CMC BW948-B" (pro)
20250402/41 : "Utilisateur CMC BW948-B" (19F_CPD)
20250402/50 : "Utilisateur CMC BW949-B" (pro)
20250402/51 : "Utilisateur CMC BW949-B" (19F_CPD)

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