FRIEDRICH-SCHILLER-UNIVERSITÄT JENA NMR-Plattform

## **Creating a sample request with SciPeaks** (May 2026)

- To reach the sample request form, open the NMR platform webpage and click on the icon "Create measurement request". If this is the first time that you submit a request to our facility, you also need to enter your SSO token (university account) to register.
- Once the SciPeaks window opens, click on the icon "**Add sample**" in the upper left side of the screen (to the right of the search field).
- Now, a window opens for the sample name definition. In the field "**Reference**", enter your user abbreviation (e.g. ABC or PPT1) which should consist of 3-4 characters. Please, only use letters and/or numbers, no space signs are admitted. Next, enter in the field "**Batch**" the sample i.d./sample name from your lab journal. Equally, only letters, numbers and hyphens are admitted (e.g. Test-10-Service). The Batch name may not exceed 16 characters. Finally, click "**Submit**".
- A new tab window appears with the name of the measurement request (Reference+Batch). Click on the icon "Molecule" to enter the (proposed) structure of the molecule in your sample. To this end, you can either use the integrated structure editor or import/upload a structure file.[2] For import, please use the icon "Import…" in the upper right corner of the editor window. Note that for each sample request, a structure is mandatory. Finally, click "**Save data**".
- Click on the "Home" tab in the upper left corner of SciPeaks: The previously generated sample should be active (green filling) – otherwise, click in the corresponding sample field.
- On the right side of the SciPeaks window (tiles area), mark the pink tile named "**NMR request**" to select the experiments for your measurements.
- The active window is now your **sample submission form**. The following entries need to be completed: Deuterated solvent (select from pull-down list "**Solvent**"), "**Weight**" (in mg), "**Temperature**" (default is 25°C), collecting point ("**Lab**" – select the sample collection cupboard where you will drop your sample), and your lab (Arbeitsgruppe, "**Group**"). In case that your sample is a polymer, please, check option "**Polymer**". Finally, you must select the NMR experiments (section "**Experiments**") which shall be recorded from your sample. If the desired experiment does not appear in the list, please, mark "**Other**" and enter the experiment name(s), which shall be recorded, in the free text field below ("**Remarks**"). The field "**Keyword**" is optional and for your own information.
- Once all fields are completed, please click in the column on the right below the "List…" field on "**Create request**". As of that moment, your request cannot be modified any longer!
- Once the request was processed by by the NMR platform, you can directly view the spectra by clicking on the corresponding sample in the "**Home**" tab and then marking the green tile "**Analyse NMR**" in the area on the right side of the window. Spectra can be downloaded by clicking on the icon "**Download raw data**".

[2] In ChemDraw, you can copy a structure by choosing „select", „edit" and „copy as" (option „MOL text")!

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