

General guidelines and rules of the OC NMR department (as of 25.07.2023)

Service NMR:

- ☐ Requests for measurements should be done through submission of a sample with a request slip
- ☐ Contact with NMR personnel preferred over the phone or by email

Self-service operation of the Open-Access spectrometer (after instruction only):

- ☐ The Open-Access Spectrometer is available to researchers of the Organic Chemistry Institute
- ☐ For instruction, please contact Timon Reckmann (timon.reckmann@wwu.de , Tel. 39773)
 - 1D NMR: ^1H , ^{19}F , ^{11}B , and ^{31}P NMR spectra (only concentrated samples!)
 - **Maximum of three samples per person at any one time**

400 MHz NMR services available on request:

- Urgent ^1H and ^{19}F NMR measurements (will be measured in priority)
(e.g. if there are too many samples in the queue of the access spectrometer!)
- ^{13}C , heteronuclear, and specialized ^{19}F NMR measurements
- Serial measurements

High-field NMR:

- Specialized 1D/2D NMR measurements – see the request slip for details
- Other specialized techniques available on request
- ☐ As a rule, only accepted after initial confirmation of purity through ^1H and ^{19}F NMR on the 400 MHz spectrometer
- ☐ **A list of all $\delta(^{19}\text{F})$ values must be given on the request slip for samples containing fluorine**

Labelling of samples:

- ☐ **No letters or symbols** should be used to label samples beyond those of the user's three-letter abbreviation, e.g.:
mue 591-1 (= **user identifier** & **reaction/sample number**)

Request slips and sample labels:

- ☐ Template should be downloaded, filled out, and printed in advance (Don't plot the paper double-sided!)
(<https://www.uni-muenster.de/Chemie.oc/en/nmr/nmr-service.html>)
- ☐ The solvent, amount of analyte, reaction number and requested experiments should be filled out by hand in legible handwriting
- ☐ One form for several samples only with the same solvent and with identical measurement requirements

Sample preparation:

- ☐ The exterior of NMR tubes must be absolutely clean
- ☐ NMR tubes must be **18–21.5 cm long**; broken or damaged NMR tubes and caps are forbidden
- ☐ Tubes should be filled to 5 cm with samples, in deuterated solvents only (**no mixtures!**)

Special case: serial measurements of x samples (where $x > 3$):

- ☐ Samples will be numbered **1 through x**
- ☐ **Only possible for samples in the same solvent and with identical measurement requirements**
- ☐ Instead of attaching a sample label, the caps should be marked 1 through x and placed in the provided sample stands (to the right of the department entrance) with one request slip per series

Sample submission and return:

- ☐ In front of the department entrance (observing all signs)

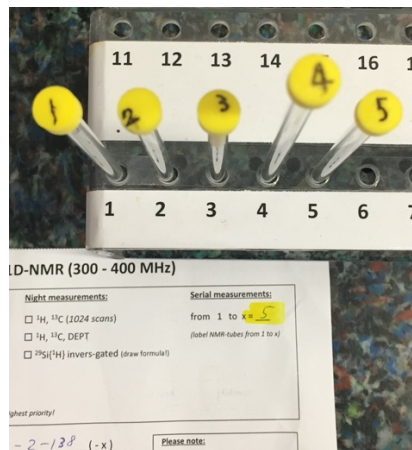
Download of raw data:

- ☐ Data from all spectrometers can be downloaded onto the user's PC immediately after measurement with the program "mora the explorer".

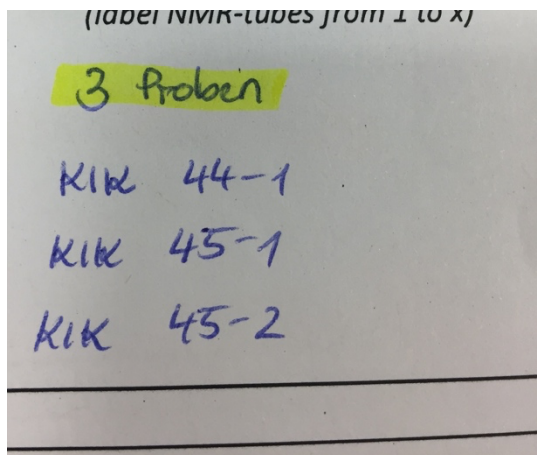
Examples:

Several samples with the **same solvent** and **identical measurement requirements**:

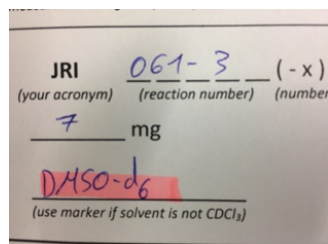
Serial measurements:
(only for more than 3 samples!)



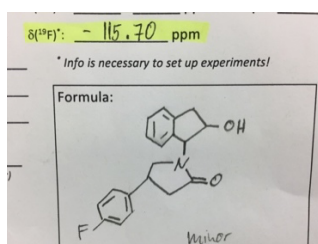
Up to three samples:
(One form, three labels)



For solvents other than CDCl_3 :



Highfield-NMR of Fluor containing compounds
list of all $\delta(^{19}\text{F})$ is required:



Acknowledgment:

We thank Matt Milner for kind translation and especially for providing the program "mora the explorer"!

Final note:

- ☐ Samples that do not conform to the guidelines 100% will be returned unmeasured.