NMR CF Data Management

Version 1.2, applicable from July 23rd, 2021

Data accessibility: The NMR CF spectrometers can only be used by CF staff or by certified users. Certification to use spectrometers is obtained by completing the course "Practical NMR spectroscopy of biomolecules (C7995)" and/or by obtaining approval by the head of CF. A unique login name is assigned to every certified user of the facility under which the users should work. New users in training can only work under a supervision of certified users or CF staff. The same logins apply to all computers of CF, namely the computers of the six spectrometers (nmr500, nmr600, nmr700m, nmr700b, nmr850, and nmr950) and nmrcf computer which is available for further processing and data manipulation. The CF computers are placed in .ncbr.muni.cz DNS domain (building C04) and are running CentOS Linux system.

Data storage: The users are provided with disk space (/d1/data) to store their data. The disk space is subject to **group quotas** assigned to research groups (RG) of 50 GB or 100 GB on spectrometers or on nmrcf, respectively. Besides that, users have small **user quotas** of 500 MB in their home directories (/home). These should be treated with caution. Filling the home quota may prevent the user from starting the TopSpin program necessary for measurement.

The computers in the NMR CF are not meant for permanent storage of the user data. The raw (ser files) and processed data should not be held for more than 1 month on the spectrometer computers and no longer than 6 months on the nmrcf computer.

All the data obtained by the users in the CF are owned by the users and it is their responsibility to transfer and archive them. The CF staff's responsibility for data measured by CF staff ends by transferring the data to the end user. The CF takes no responsibility for loss of data measured by non-staff users.

Data transfer: The preferred way of sharing the data with external users is the FileSender service. For storing the data for longer time periods, the data storages offered by MU/CESNET can be used. Users can also access the spectrometers remotely via SSH from selected subnets of MU network and transfer their data directly to their work computers via SCP/SFTP.

Data security: The users can view/copy other users' data but should not do so without prior consent of the data owner. The default permissions additionally allow all group members to (over)write or delete the data within their research group – this enables the group to manage their data even if a user leaves the group. The data (over)writing is not allowed between groups. **Handling of sensitive data** is possible by setting file/directory permissions accordingly by the users themselves or by the CF staff upon request.

Destruction of old data: The CF staff can handle other users' data for the purpose of computer maintenance and backup. If necessary, the CF staff will remove old files to free the disk space, after a prior warning, or even without a warning in emergency if the data would prevent the use of the spectrometer or computer. No data will be intentionally lost in the process.

Backup: The NMR data, user homes, and the TopSpin directory on the spectrometers are synchronized with the backup disk every night, the old copies are overwritten. The NMR data and user homes on the nmrcf computer are stored on 2-disk RAID1/mirror, so the data synchronization is done in real time and the system works even if 1 of the disks fails.

Responsible person from CF: The person responsible for the data management in the NMR CF is Mgr. Petr Padrta, PhD.