

Terms of use „Center for Structural Studies (CSS)“

The „*Center for Structural Studies*“ is a central scientific research and service facility of the Faculty of Mathematics and Natural Science at the Heinrich-Heine-University Düsseldorf within the area of structure-supplying methods, especially to determine the three-dimensional structure of proteins by means of X-ray diffraction analysis (MX) or to resolve the in-solution-structure of proteins and complexes using Small-Angle-Light-Scattering (SAXS).

The aim of the CSS is to enable all interested users guided access to our infrastructure (special chemicals and crystallization equipment, devices, synchrotron beam time) and scientific support for the individual experiments of all members of the HHU and external users. The CSS provides all steps (protein crystallization, crystal optimization, search for suitable cryo conditions, data collection, structure determination and refinement) as full-service as well as hands-on support.

Responsible, authorized staff:

Executive director: Prof. Dr. Sander Smits

Operating leader: Dr. Astrid Port

Associate: Jens Reiners

§ 1 Instructions

All devices except pipetting robot and X-ray generator can only be used independently after an introduction by an authorized person. Application related settings are allowed to be modified by the user, whereas fundamental settings and configurations must not be changed.

Synchrotron measurements are only performed by the authorized personnel.

§ 2 Liabilities

For all damages to devices, pipettes or other tools, which are verifiable caused by misuse, the user or the corresponding institutes head is liable. They have to incur any expenses for repairing. The responsible staff of the „*Center for Structural Studies*“ is authorized to exclude users from any further application.

§ 3 Duty to report specific incidents

In case of software issues, error messages, broken devices or similar, the user has to stop working immediately and is obligated to quickly report the responsible administrator. It is strictly forbidden to perform repairs or adjustment independently.

§ 4 Appointments

For crystallization trials requiring the pipetting robot, for diffraction measurements with the X-ray generator or the SAXS measurements the user has to arrange an appointment with the responsible personnel at least two days in advance. In every case the user is obligated to agree with the responsible person to get access to the labs in order to ensure smooth operations flow. All projects are processed one after another or according to the corresponding appointment, respectively.

§ 5 Data storage and backup

Data must only be stored temporarily in the dedicated folder of the controlling computer (mostly in folder „User“). It is strictly forbidden to connect own storage media to the controlling computers without agreement of the responsible personnel. For backup of the own data the user is self-reliant. All data on the controlling computers are reviewed regularly and, when necessary, deleted by the administrators. All data collected at synchrotrons are stored on a appropriate backup server by the administrators.

§ 6 Usage of data and image material in publications

If data or images, which were generated on devices of the CSS or collected at synchrotrons as service, are used in publications of a research group, the „*Center for Structural Studies*“ should be mentioned in the acknowledgements.

All users of the CSS must acknowledge the DFG in their publications:

"The Center for Structural Studies is funded by the Deutsche Forschungsgemeinschaft (DFG Grant number 417919780)."

For X-ray diffraction data please mention also „INST 208/740-1 FUGG“ (X-ray diffractometer), for SAXS data „INST 208/761-1 FUGG“ (SAXS machine).

Furthermore, the CSS responsables should be informed. The results obtained are only provided to the client, transfer to third party only with explicit permission of the client.

§ 7 Charges and fees

All users have to participate in costs for wear and tear. This could be done either by paying an annual membership fee or by a surcharge of the used consumables.

Groups	Membership fee p.a.
Single groups	700 Euro
GRK's	2 000 Euro
SFB's	2 500 Euro
Cluster of Excellence	3 000 Euro
External groups	1 000 Euro

For all various experiments or used consumables different costs incur. These costs for consumables (plates, chemicals etc.) depend on the corresponding current purchase prices and may underlie annual changes. The settlement is made half-yearly based on the consumables etc. spent. The permission of any user to use the „Center for Structural Studies“ has to be given in writing by the corresponding head of the institute or other budget responsible person.

§ 8 Sample preparation protein crystallization

To ensure an optimal screening and a good reproducibility some aspects are of importance and some documents/chemical agents are needed (see also order from):

- 1.) the low molar protein buffer should contain as less agents as possible (just as much as is required for protein stability; if possible avoid phosphate buffer)
- 2.) protein need to be pure (at least 90 % on SDS-PAGE), and homogenous (only one oligomeric state)
- 3.) protein has to be stable over at least three weeks (at 4 °C, 12 °C or 20 °C)
- 4.) protein concentration at least: 5 – 10 mg/ml
- 5.) minimum protein volume per screen (96 conditions): 15 µl
- 6.) please include in the delivery about 2 ml protein buffer with declaration of all ingredients

Furthermore some information is essential for our experiments:

- 7.) please declare date of the protein purification and storage/stability conditions
- 8.) please attach image SDS-

- 9.) homogeneity verification (please attach e. g. image gel filtration)
- 10.) please provide protein concentration, molecular weight and composition of the protein buffer
- 11.) if the protein requires certain ligands (like metal ions, cofactors etc.) for activity and/or stability, please state
- 12.) is there an activity assay? If so: please ensure that the protein is still active in the used buffer? In case of co-crystallization trials: please state the substrate(s) and suitable concentration(s). Include the substrate(s) in the delivery unless they are commercially available.

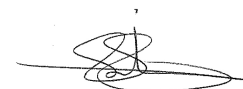
§ 9 Sample preparation SAXS measurements

For a planned SAXS measurement, some aspects are of importance and some documents/chemical agents are needed (see also [order form](#)):

1. the low molar protein buffer should contain as less agents as possible (just as much as is required for protein stability; avoid phosphate buffer and more than 5 % glycerol)
2. protein needs to be pure (at least 95 % on SDS-PAGE), and homogenous (only one oligomeric state)
3. protein has to be stable over at least two days (at 4 °C, 12 °C or 20 °C)
4. protein concentration at least: 5 - 10 mg/ml
5. minimum protein volume per measurement: 70 µl
6. please provide about 2 ml protein buffer with declaration of all ingredients. (Important: It has to be exactly the same buffer used for the protein purification/dialysis/concentration for proper intensity determination!)

Furthermore, some information is essential for our experiments:

1. date of the protein purification and storage/stability conditions
2. image of SDS-PAGE
3. homogeneity verification (e. g. gel filtration)
4. protein concentration, molecular weight, extinction coefficient and composition of the protein buffer
5. if the protein requires certain ligands (like metal ions, cofactors etc.) for activity and/or stability, please state
6. Protein sequence including purification tags and cleavage sites (text file)
7. If available: structure or homology model



Prof. Dr. Sander Smits