Current State and prospects of the Small Angle Neutron Scattering Spectrometer YuMO

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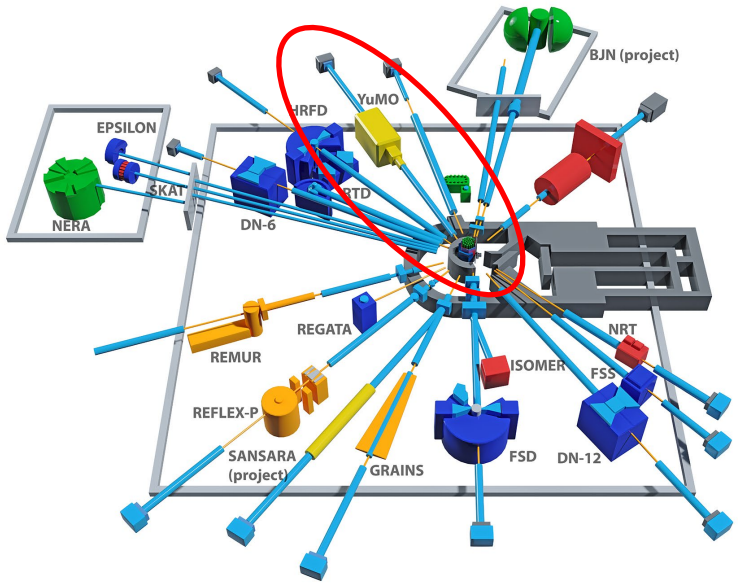
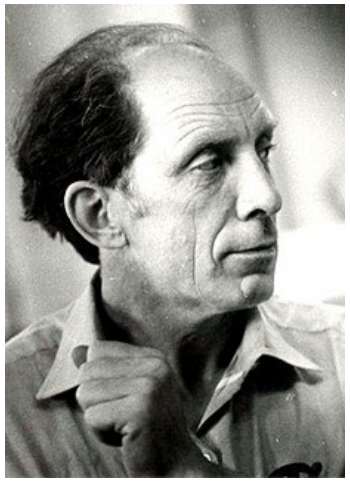
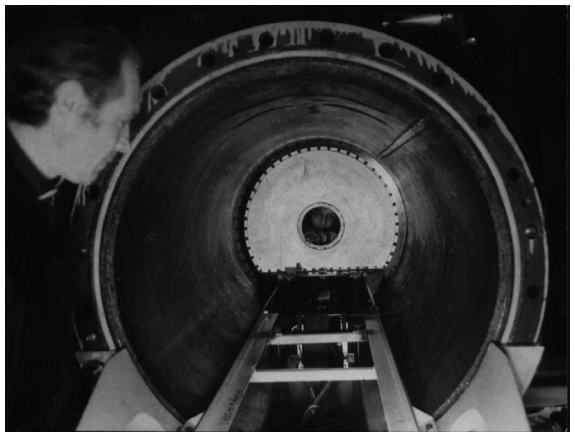
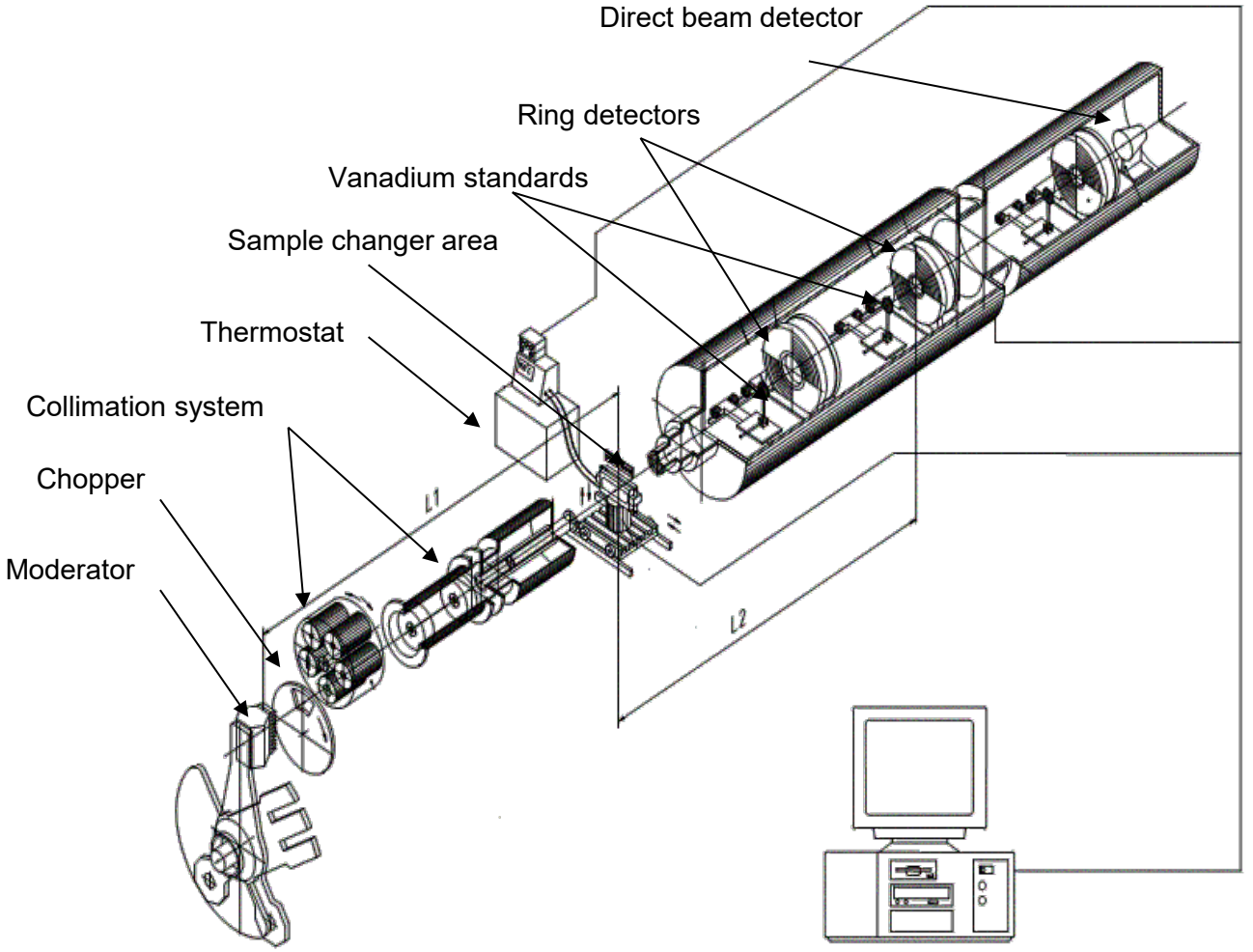
61th meeting of the PAC for Condensed Matter Physics

YuMO spectrometer









Kuklin, A.I., Ivankov O.I., Rogachev A.V., Soloviov D., Islamov A., Skoi V.V., Kovalev Y., Vlasov A., Rizhikau Y.L., Soloviev A., Kucerka N., Gordeliy V., *Small-Angle Neutron Scattering at the Pulsed Reactor IBR-2: Current Status and Prospects.* Crystallography Reports, 2021. **66**(2): p. 230-241.

YuMO spectrometer

Since February 17 to April 25 (3 reactor cycles)

- **About 30 scientific experiments** including test experiments and fast proposal experiment **were done** (Moscow, St.-Petersburg, Volgograd, Dolgoprudny, Dubna in collaborations with others)
- Methodological experiments and works:
  - **the collimator system and chopper adjustment;**
  - tests of the **new electronics for the Positional Sensitive Detector;**
  - implementation of **upgraded Direct Beam Detector;**
  - the instrument **electronics commissioning** after instrument long shutdown;
  - programs test and updates.

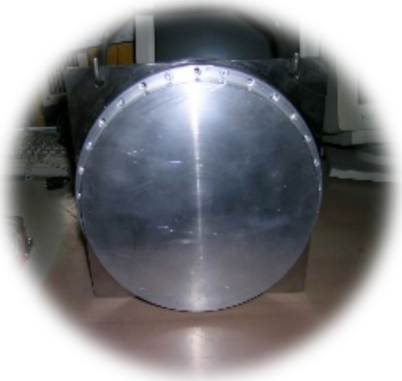
35 proposal were submitted for the second part 2025 (33%)

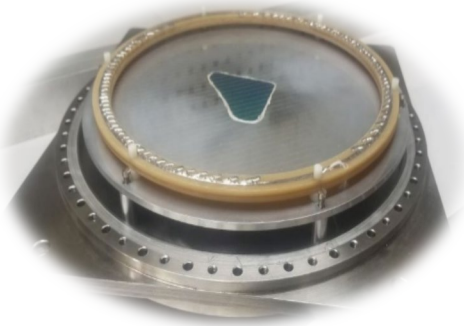
Main parameters of the YuMO spectrometer

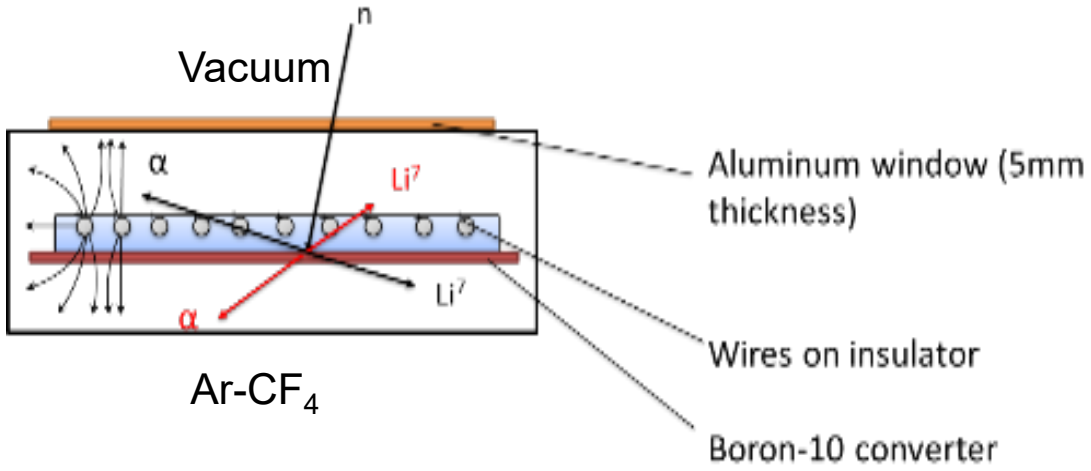
Parameters	Value
Flux on the sample (thermal neutrons)	$10^7 \div 4x10^7$ n/(s cm^2) [1]
Used wavelength	0.7 Å to 8 Å (10 Å with 30K cold moderator)#
Q-range	$7x10^{-3} \div 0.5$ Å^{-1} (~$4x10^{-3} \div 0.5$ Å^{-1})
Dynamic Q-range	q_{max}/q_{min} up to 100
Specific features	Two detectors system, central hole detectors
Accessible size range of the structural features under investigation *	1000 ÷ 10 Å
Intensity (absolute units -minimal levels)	0.01 cm^{-1}
Calibration standard	Vanadium during the experiment
Beam dimension at the sample position	14 mm diameter
Collimation system	Axial
Detectors	^{3}He filled, 8 independent wires, in-house design
Detector (direct beam)	^{6}Li-convertor in-house design
Sample changer	Placed in the custom made box, in air
Q-resolution	low , 5-20%
Temperature range	4°C - + 70°C (standard Hellma cells, 1mm, 2mm pathlength) -20°C - + 130°C (custom designed sample holders required)^
Number of the samples in the automated sample changer	25 ***
Background intensity	0.03 – 0.2 cm^{-1}
Average single seta data collection time	1 h
Source pulse frequency	5 Hz
Control computer Operating system	WINDOWS 10
The instrument control software suit	SONIX
Controlling parameters	Starts (time of experiments), power, vanadium standard position, samples position, samples changer temperature, vacuum level in the detectors tube .

Direct Beam Detector Upgrading

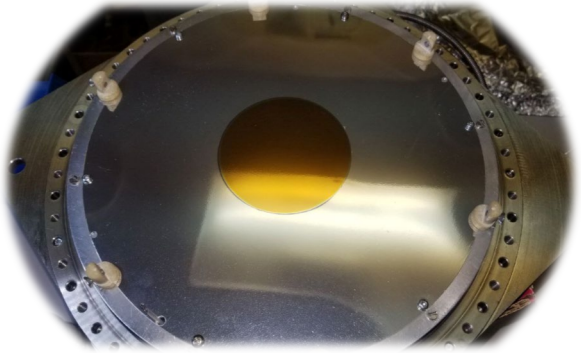
Old (2011-2021) B^{10} converter





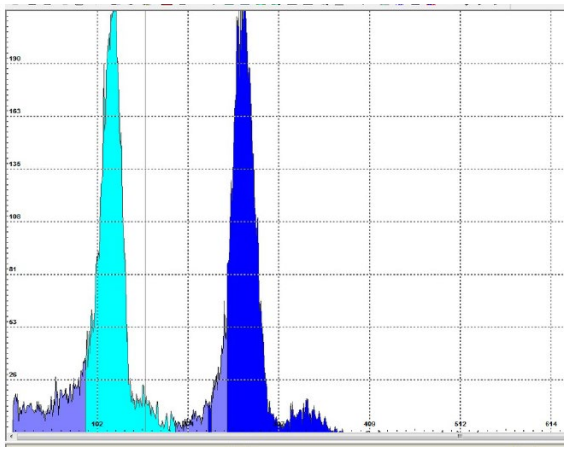


New B^{10} converter



Sensitive area Ø=80 mm, thickness=60nm
Ar/CF_4 (94/6%), 900 mbar

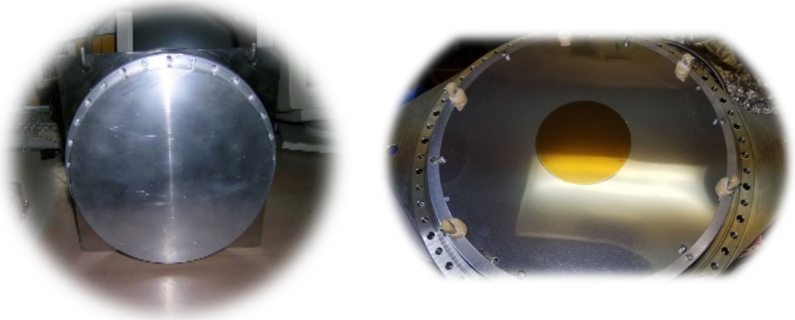
Amplitude spectrum

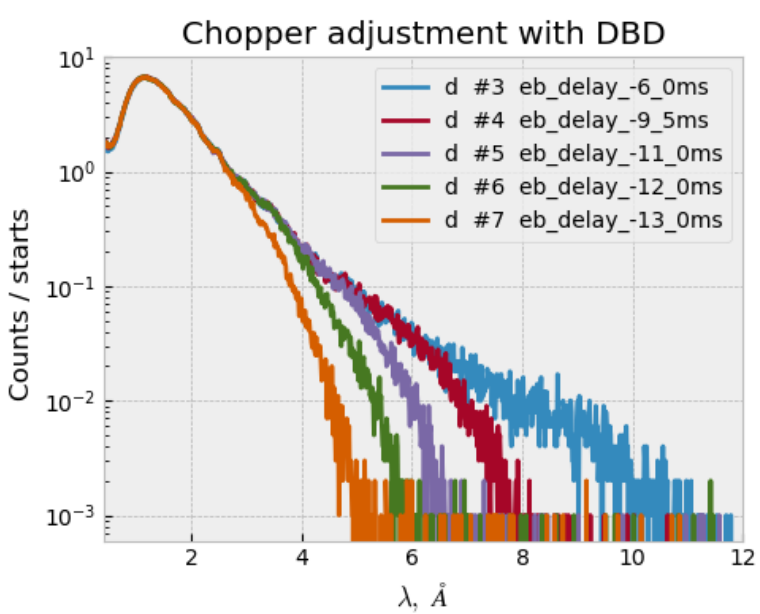


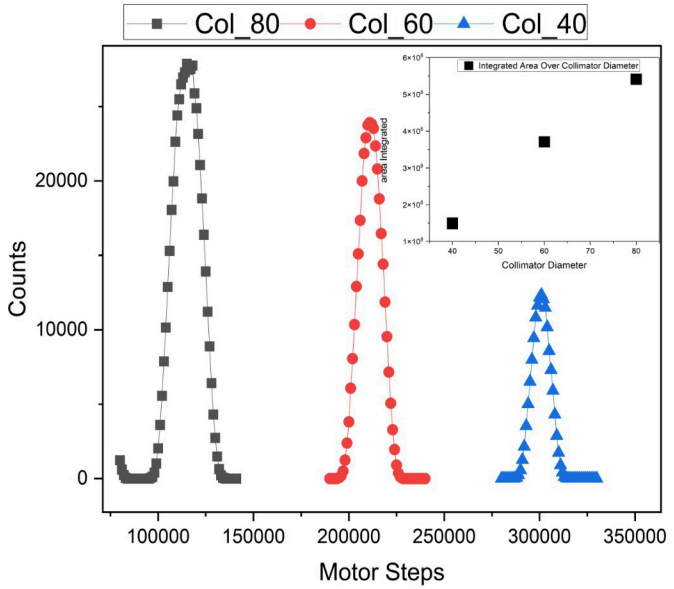
$$n + {}^{10}B \rightarrow \begin{cases} \alpha + {}^{7}Li + 2.792MeV, 6.1\% \\ \alpha + {}^{7}Li^{*} + 2.310MeV, 93.9\%. \end{cases}$$

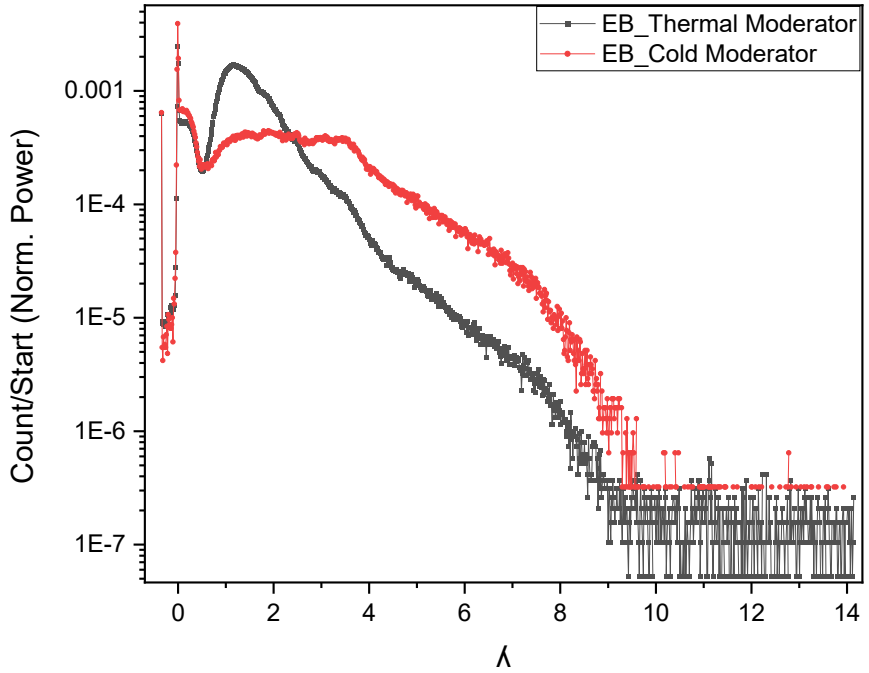
$${}^{7}Li^{*} \rightarrow {}^{7}Li + \gamma + 0.478MeV$$

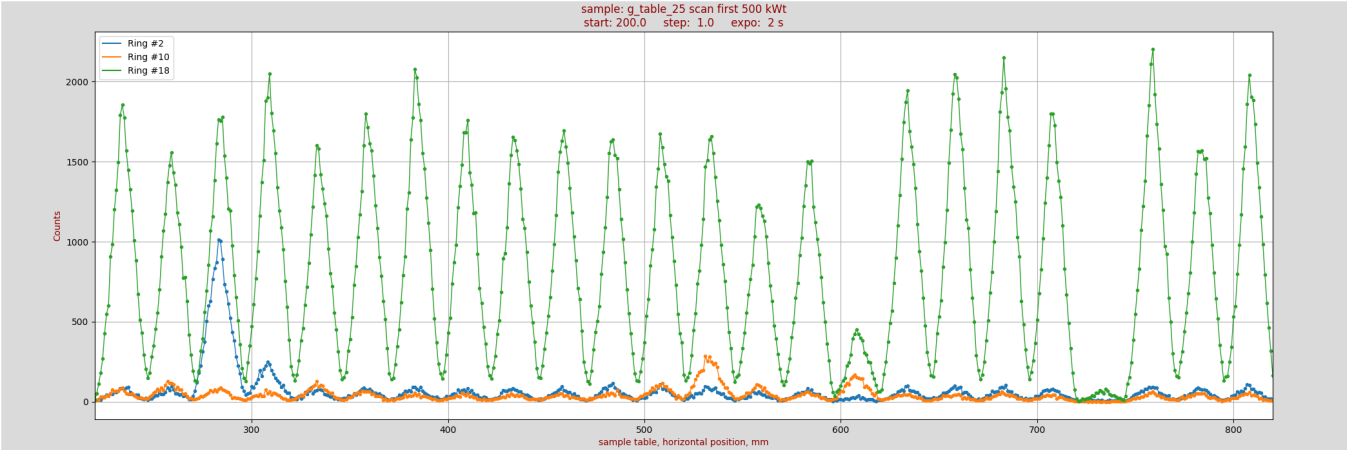
Direct Beam Detector Upgrading



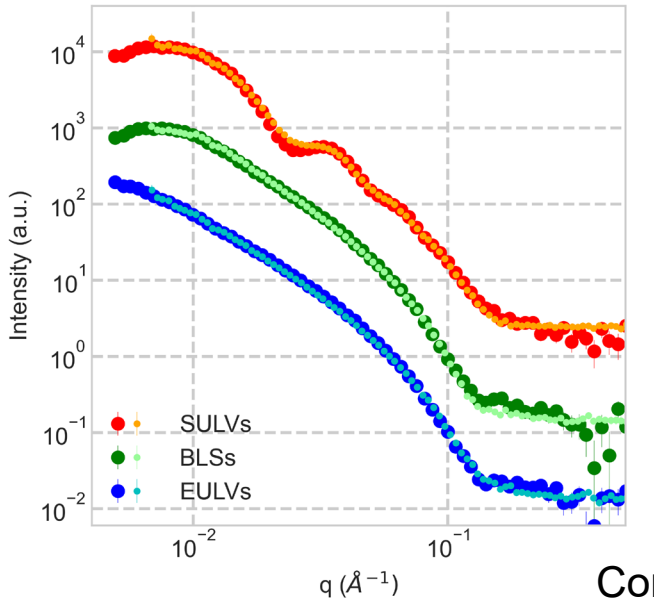






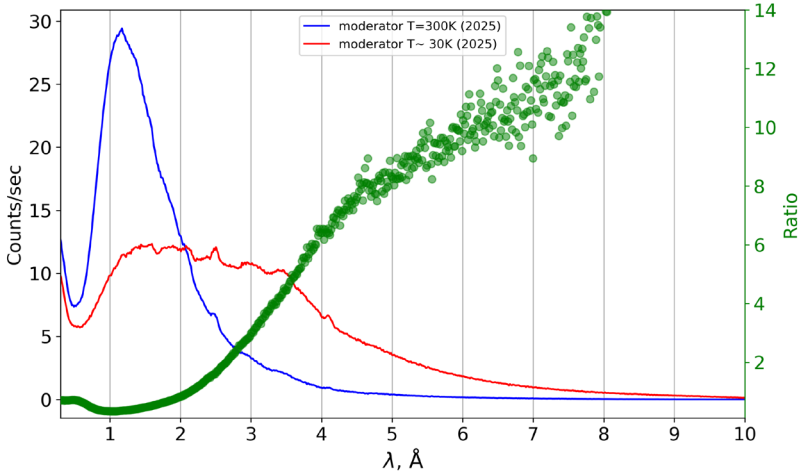


Cold moderator implementation

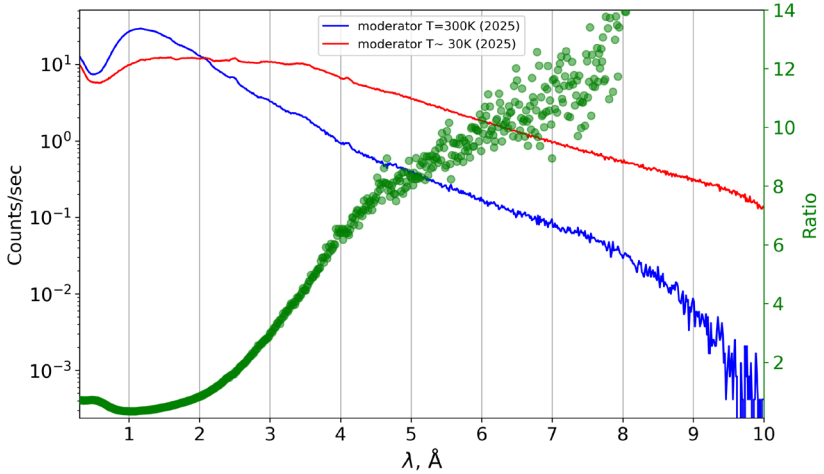


The low-q enhanced data (large circles) compared to the data of standard setup (small circles). The different forms of scattering curves allow to distinguish the overall shape of membrane organization (SULVs vs. BLSs vs. EULVs).

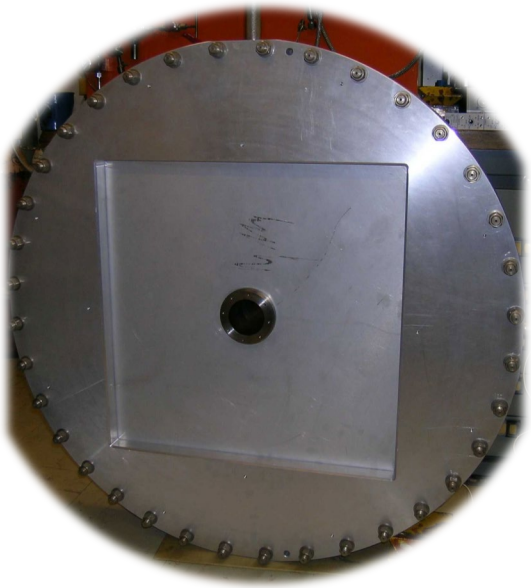
Comparison of the counts on the detectors with the cold moderator at ~ 300K and ~30K



Gain Factor (Ratio):
min ~ 0.3 (1.5 Å)
max ~ 12 (> 5Å)



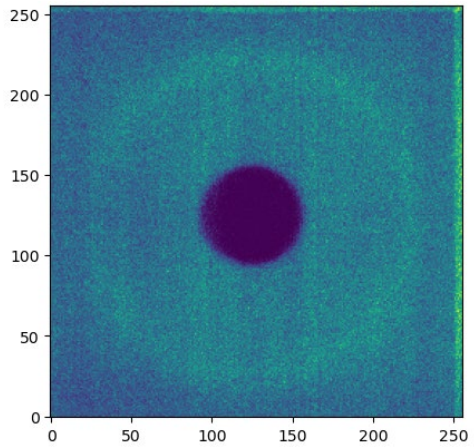
New data acquisition electronics for YuMO PSD Detector

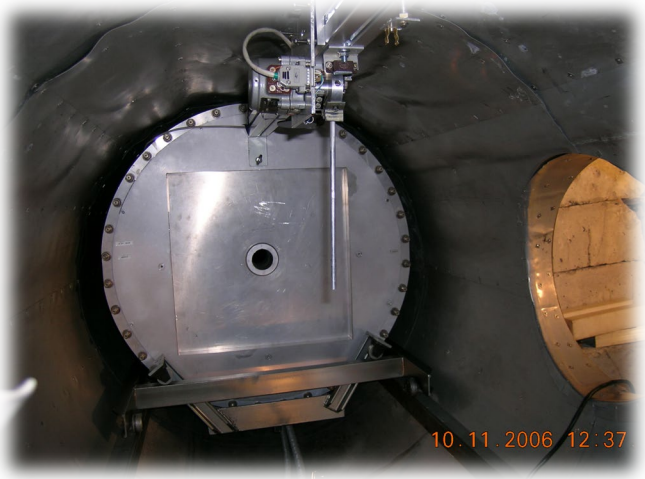


Detector mechanical parameters characteristics:

External diameter:	1070 mm
Central hole diameter:	70 mm
Body material:	Aluminum
Window thickness:	8 mm
Detection depth:	40 mm
Sealing type:	O-ring (outer and inner) and Cu-ring for conflats
Weight:	181 kg

Spectrum from the AgBe.





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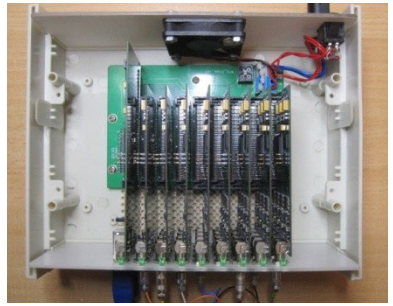
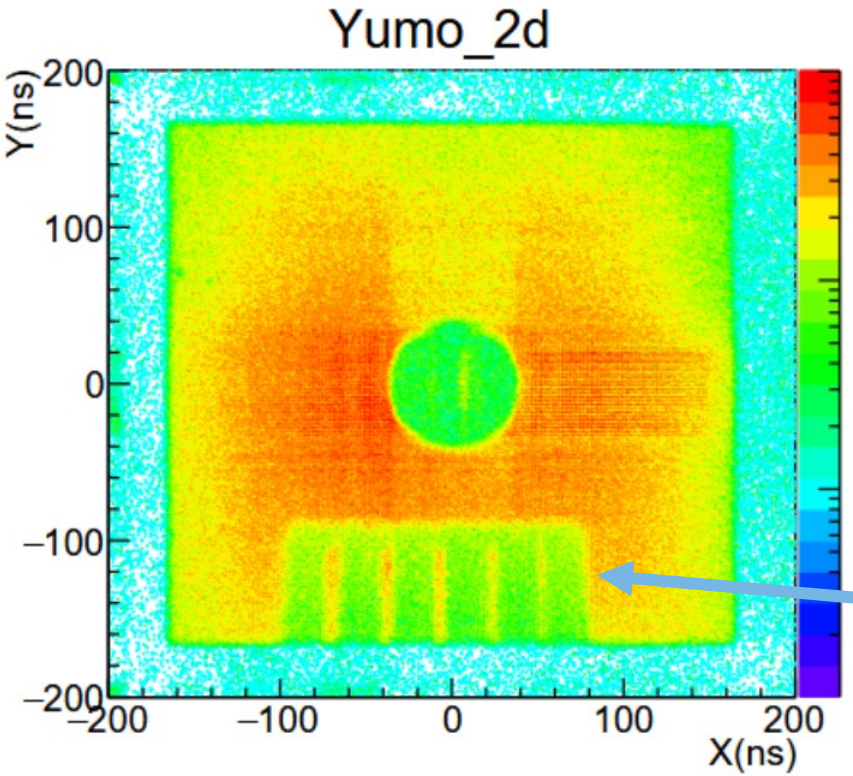
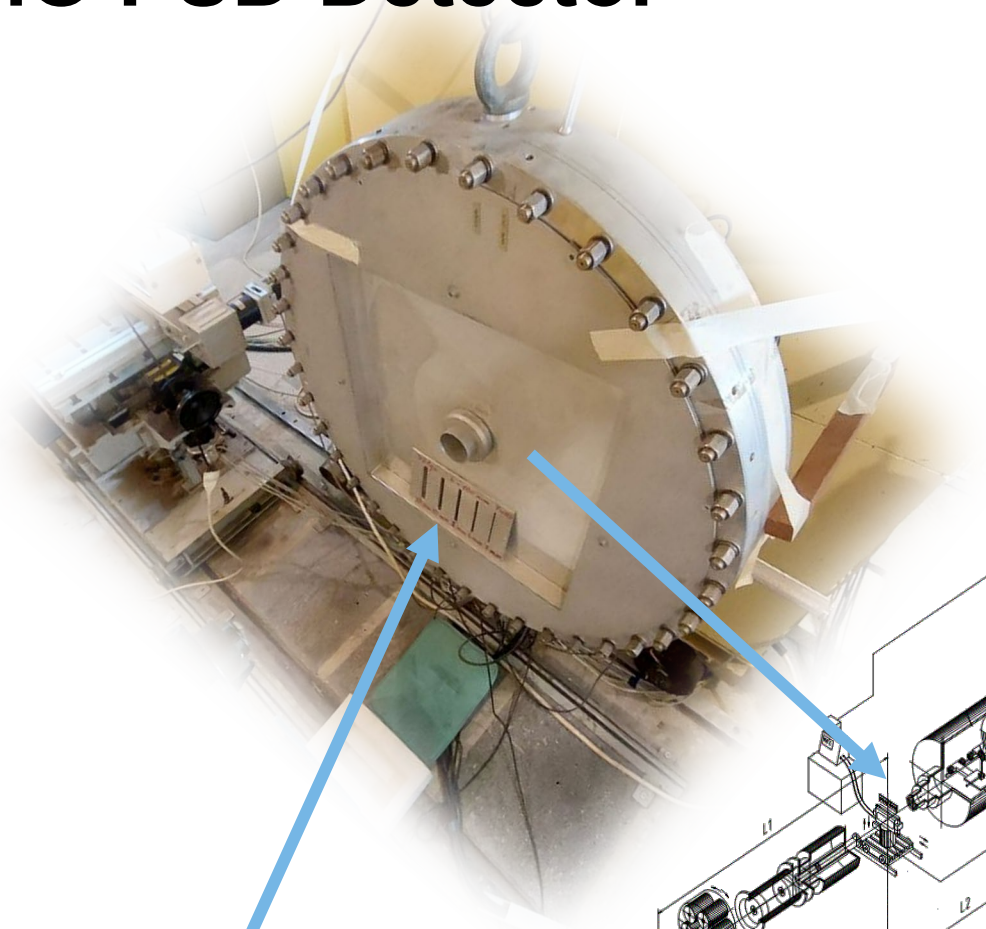
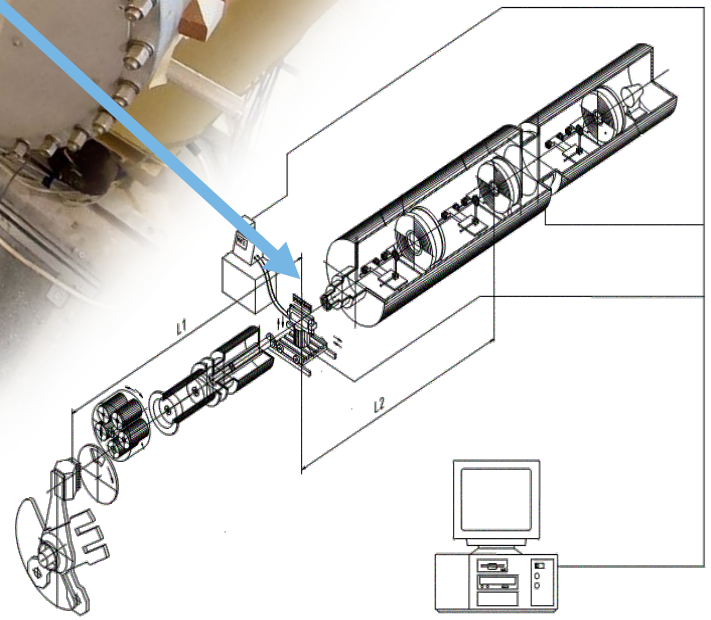




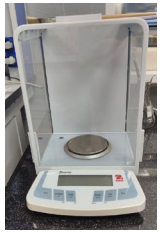


Cadmium mask.



Remote PC

Sample preparation room



Responsible: T. Murugova

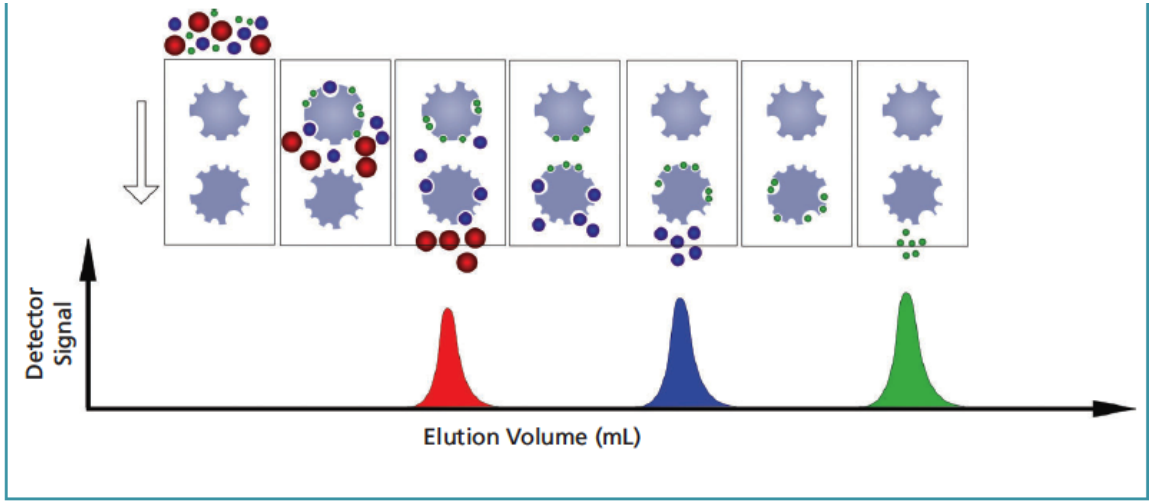
https://ibr-2.jinr.int

Size-exclusion chromatography (SEC)

Applications:

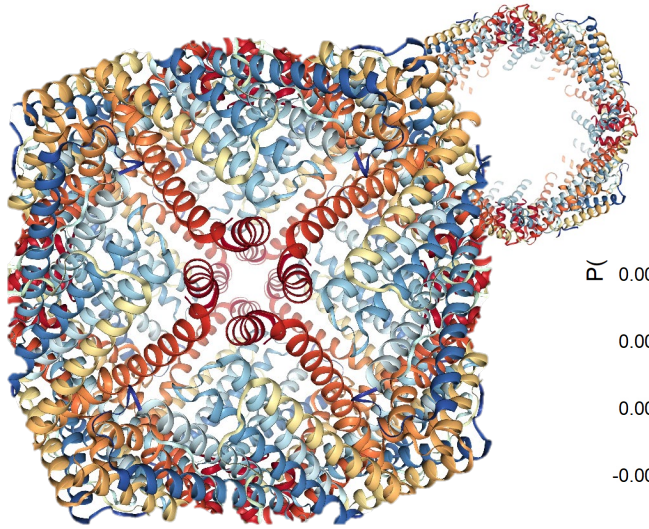
- Separation of macromolecules from complex mixtures according to their size, charge, selective non-covalent interaction and other properties.
- Protein and polimers purification.
- Affinity-tagged protein purification.
- Desalting and buffer exchange.
- Identification and quantitation of macromolecules (evaluation of hydrodinamic size of a macromolecule).
- Detects the unknown compounds and purity of mixture.

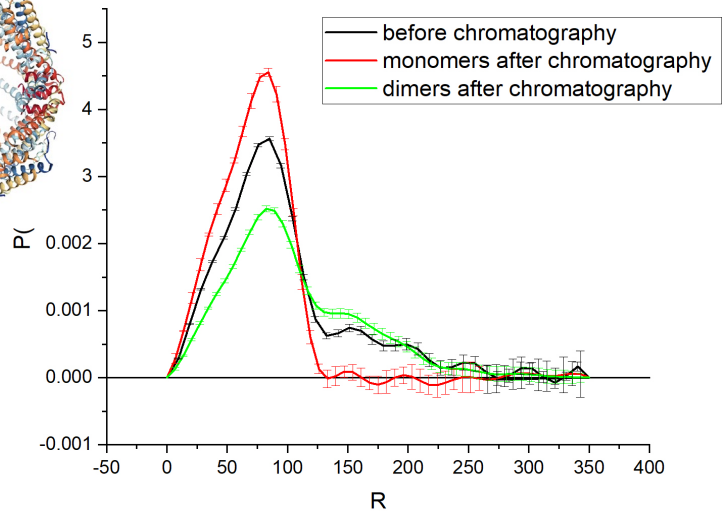
Funding:
- RSF Grant (Kucerka N.)
- Department of Spectrometers Complex IBR-2 (Kulikov S., Bodnarchuk V.)
- JINR-Poland Grant (Kuklin A.)

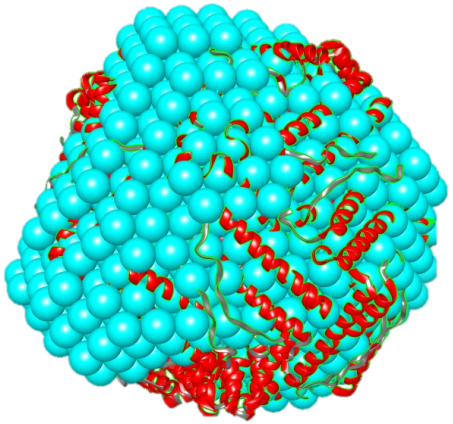


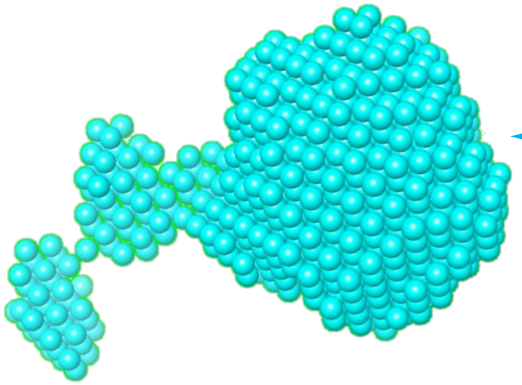
Implementation of SEC on YuMO spectrometer

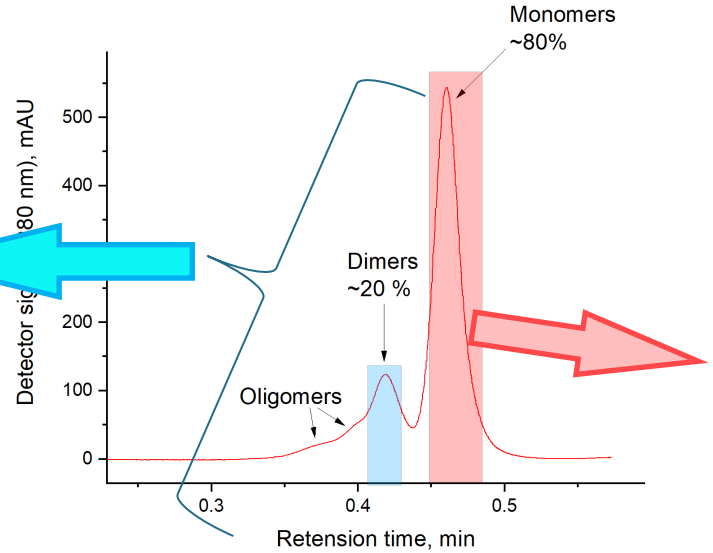
Apoferritin protein

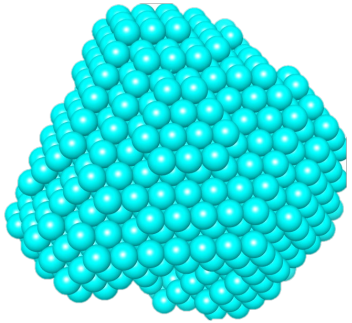












D. I. Svergun (1999) Restoring low resolution structure of biological macromolecules from solution scattering using simulated annealing. *Biophys J.* 2879-2886

Spectrometer upgrades

Spectrometer upgrade:

- Upgrade of the direct beam detector;
- Implementation of new electronics for position sensitive detector (in future for all detectors);
- Detectors adjustment in vacuum tube;
- Reconstruction of the collimating base:
  - New vacuum system;
  - Reconstruction of changeable collimator;
- Reconstruction of the sample table and holders

Programs for data acquisition and data treatment:

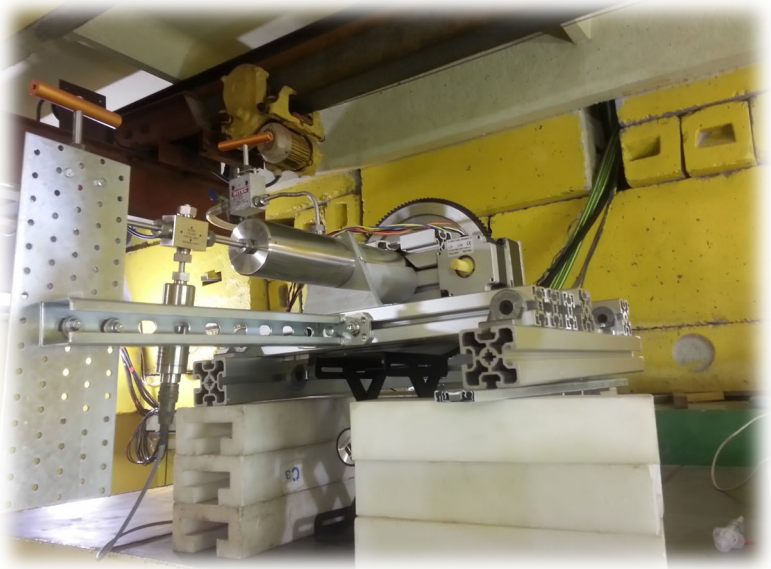
- Upgrading of Sonix+ program complex for:
  - Implementation of new electronics;
  - Implementation of FLNP file server for data storage;
- Updating of SAS program for data treatment;
- Upgrading program for data treatment from position sensitive detector

Sample holders for YuMO spectrometer

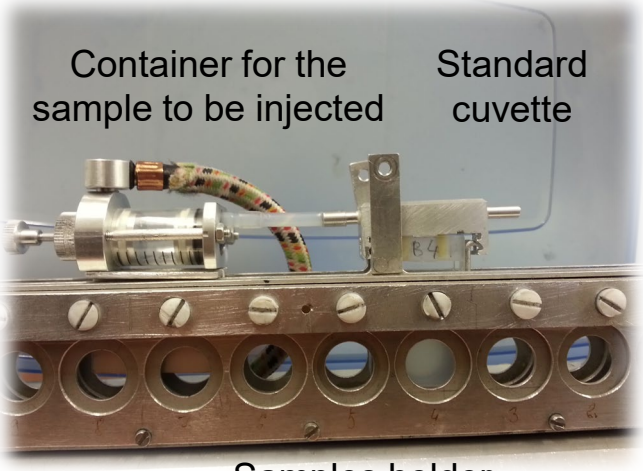
25 samples holder with connected Lauda liquid thermostat

Magnetic system

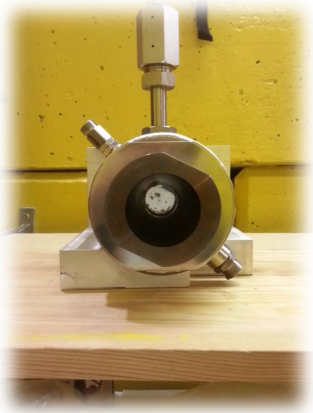
Volumetric system



Kinetics system for YuMO spectrometer



Samples holder



Acknowledgments

YuMO group

FLNP:

Kopach Yu.N.,

Kirilov A.S., Petukhova T.B., Murashkevich S.M., Morkovnikov I.A.

Bodnarchuk V.I., Bogdzel A.A., Churakov A.V., Kurilkin A.K.,

Milkov V.M., Kolesnikov A.G., Altynov A.V., Zernin N.D.,

Chernikov A.N.

LIT:

Solovjev A.G., Solovjeva T.

LHEP:

Enik T.L.

DLNP:

Kutuzov S.A.

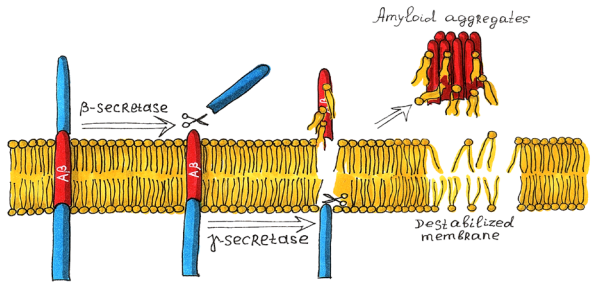
FLNP User policy group

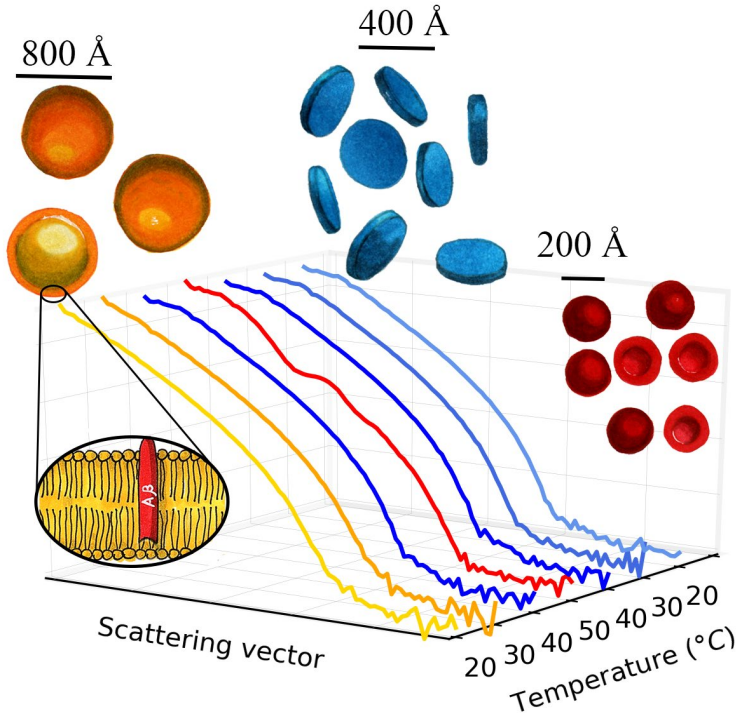
FLNP Directorate

FLNP Department of Neutron Investigations of Condensed Matter

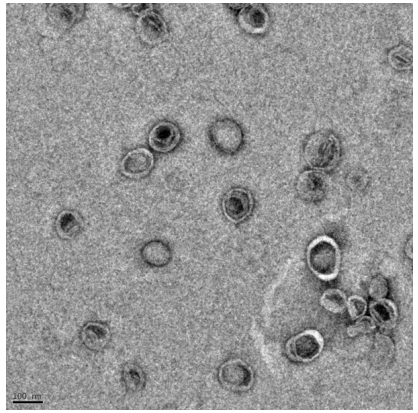
Thank you for your attention!

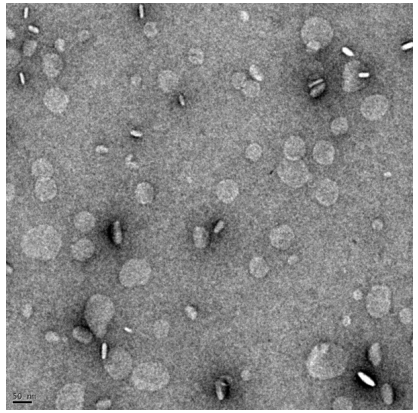
Interactions in Disease Modeling Membranes





Neutron scattering allows to study model membranes that replicate pre-clinical conditions of **Alzheimer's disease**





TEM images of the DMPC (left) and DMPC/Aβ25-35 (right) systems collected at 20° C. The dark bars (100 and 50 nm, respectively) in the lower left corners allow to assess the length scales. Objects in the left-hand panel match the typical vesicular objects with mostly unilamellar walls. The right-hand panel reveals randomly oriented discs also consisting of single layers.

Changes in the membrane self-organization happen during the thermodynamic phase transitions of lipids and are interpreted as the **peptide driven membrane damage**.

O. Ivankov, T.N. Murugova, E.V. Ermakova, T. Kondela, D.R. Badreeva, P. Hrubovčák, D. Soloviov, A. Tsarenko, A. Rogachev, A.I. Kuklin, N. Kučerka , *The Journal of Physical Chemistry Letters (under review)*

Kinetics system for YuMO spectrometer

Time of measurement – 2 min

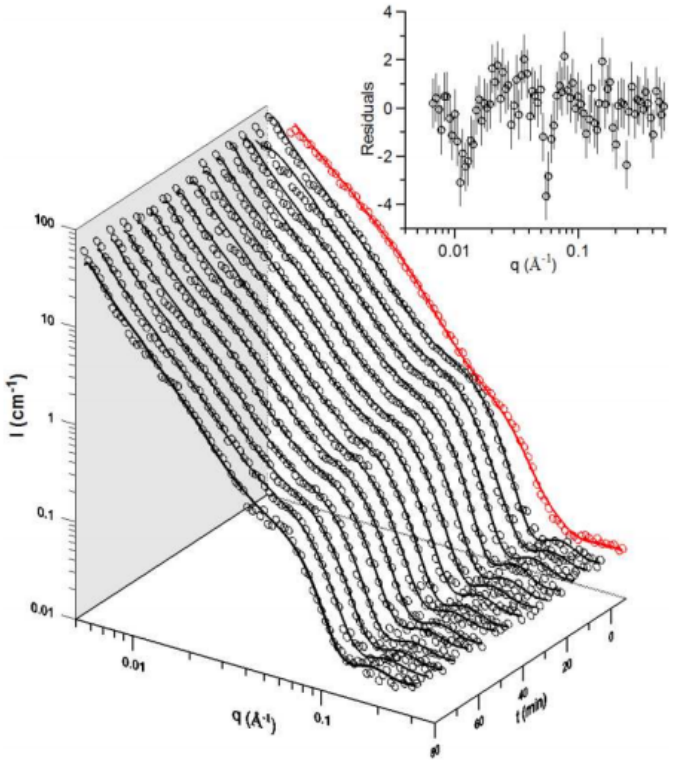


Figure 4. Dependences of SANS intensity *I(q)* on scattering vector *q* for DNA – C_{12}NO/DOPE dispersion as a function of time; prior (red points) and after DCl injection. Full lines show fits using a paracrystal lamellar model.
Inset: An example of the distribution of residuals.

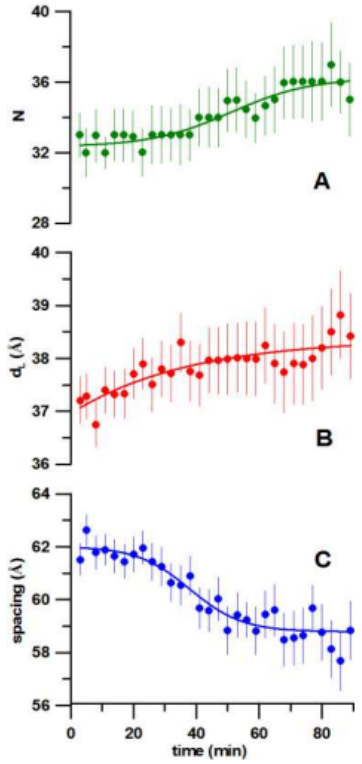
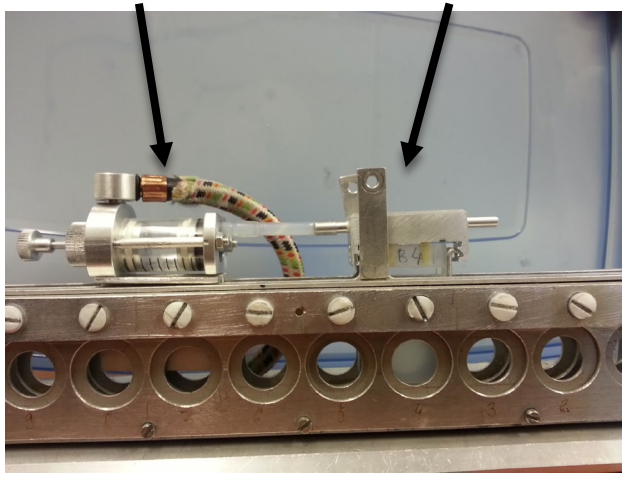


Figure 5. Time dependence of the structural parameters: the number of layers (A), the lipid bilayer thickness (B) and the spacing (C).

Container for the sample to be injected

Standard cuvette

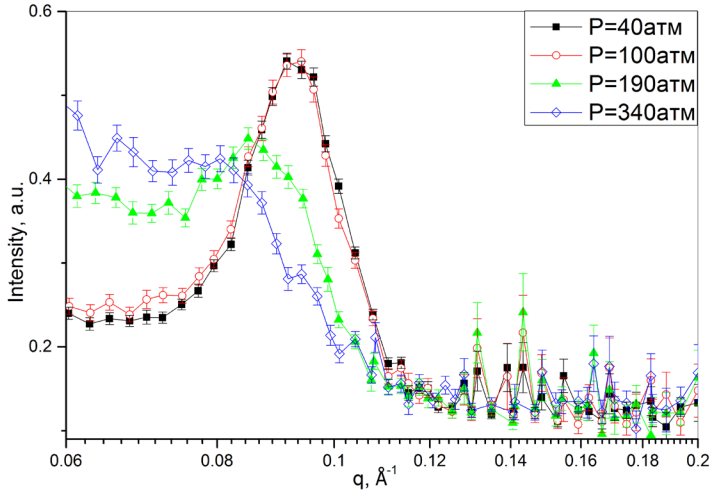


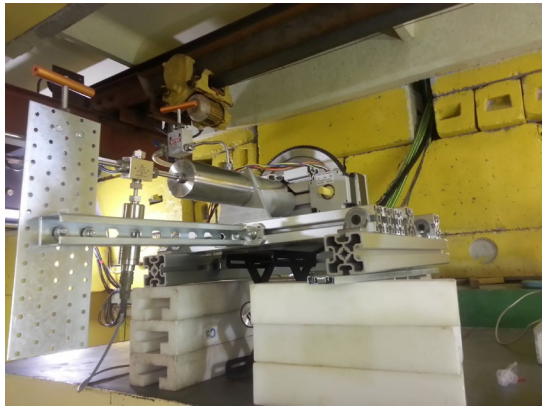
Samples holder

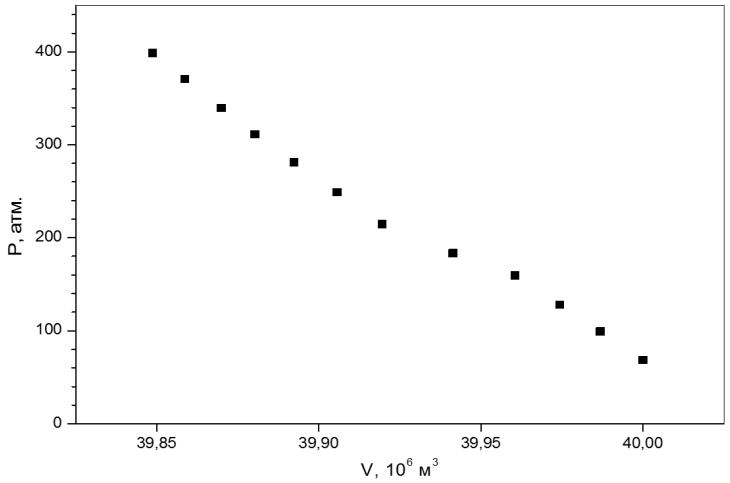
Kinetics system was developed and manufactured in Commenius University of Bratislava, Slovakia

D. Uhríková, J. Teixeira, L. Hubčík, A. Búcsi, T. Kondela, T. Murugova, and O. I. Ivankov, Journal of Physics: Conference Series **848,** 012007 (2017).

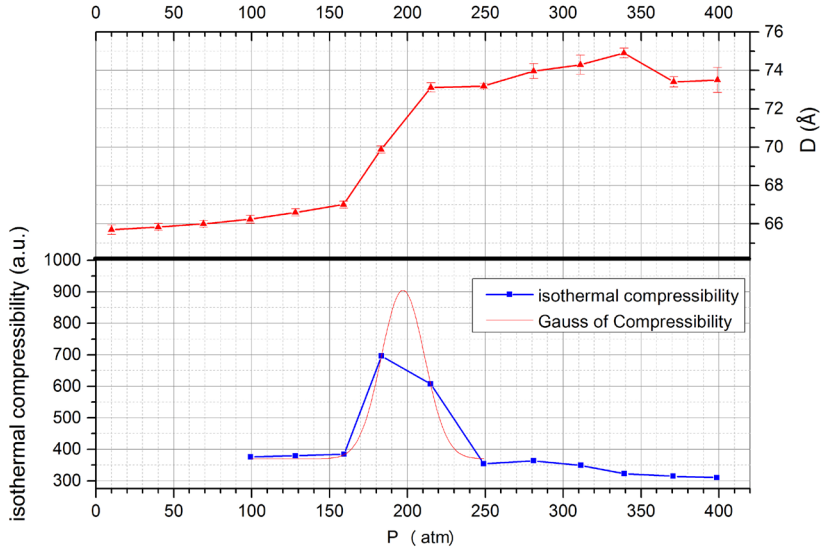
Volumetric setup for YuMO spectrometer







- Volume of the sample required: 3-4 ml
- Pressure up to 2 kBar



Soloviov, D., et al., *Changes in the Area per Lipid Molecule by P–V–T and SANS Investigations.* Macromolecular Symposia, 2014. **335**(1): p. 58-61.