

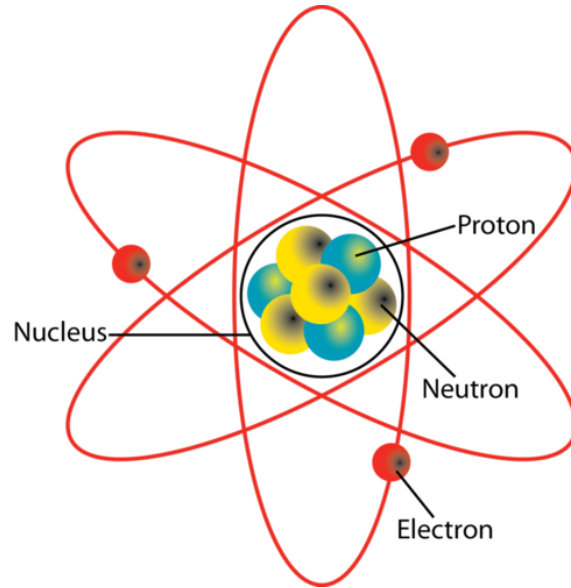
Challenges of a SANS experiment

Anne MARTEL, D22, LSS group

Introduction:

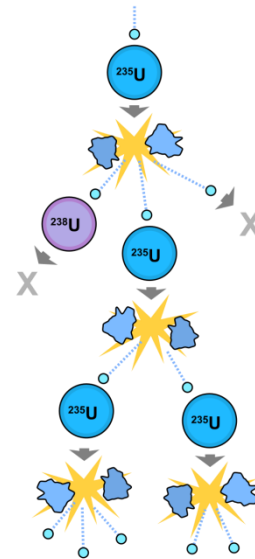
Neutrons:

Neutrons are part of the nucleus of any atom.

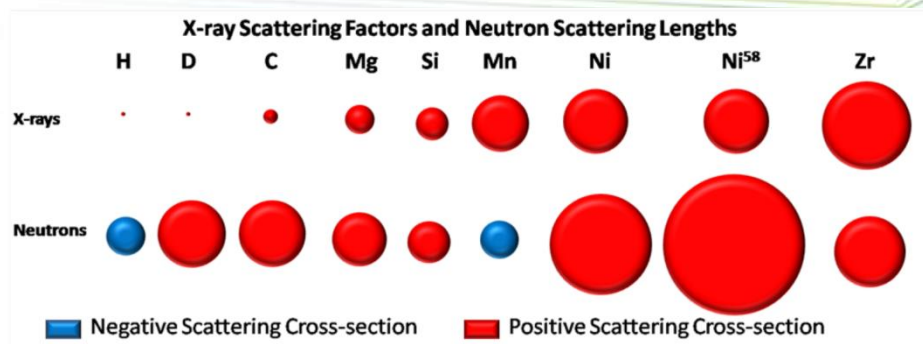


Main strength: Neutrons “see” hydrogens.

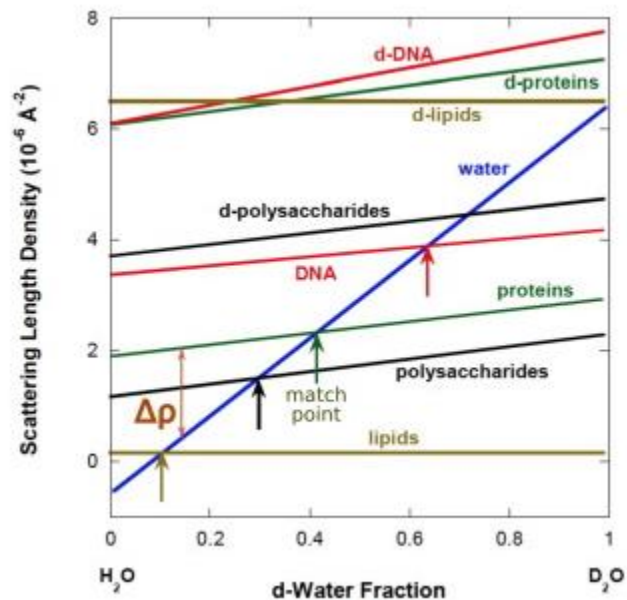
ILL, the European neutron source, produces neutrons by nuclear reaction



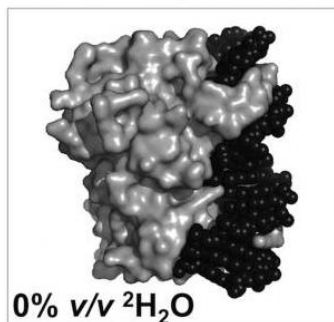
Neutrons vs X-rays: Contrast Variation



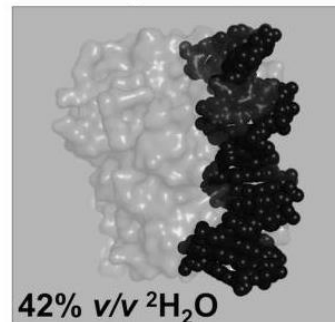
<http://www.ncnr.nist.gov/resources/n-lengths/>
http://www.isis.rl.ac.uk/ISISPublic/reference/Xray_scatfac.htm



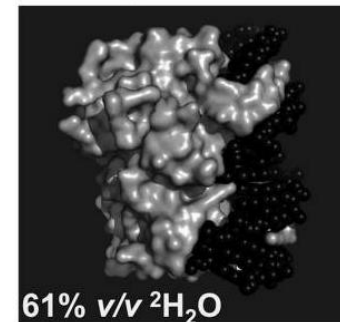
**Protein/DNA
Complex**



**Protein match
point**



**DNA match
point**



Castellanos et al., Computational and Structural Biotechnology Journal (2016)
 Jeffries et al., Nature Protocols volume 11, pages 2122–2153 (2016)



$$Q = 4 \pi \cdot \sin\theta / \lambda$$

From LLB

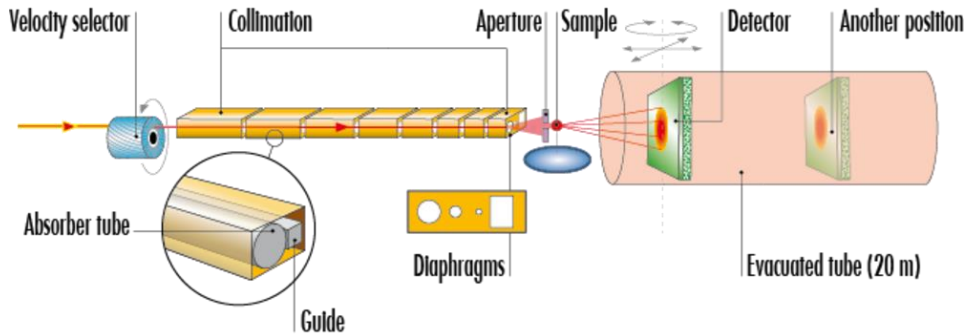


D11 description:

https://www.ill.eu/fileadmin/user_upload/ILL/3_Users/Instruments/Instruments_list/00_-_LARGE_SCALE_STRUCTURES/D11/html5/D11-principle/D11.html

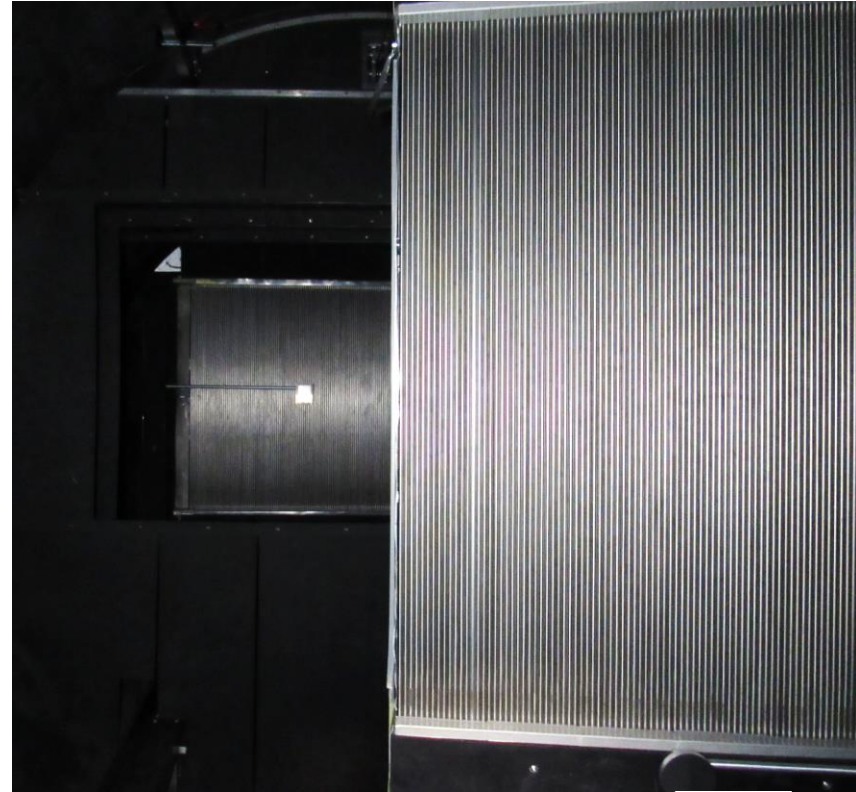
A. Filhol

D22 ++



2nd detector > whole Q-range in one set up
Semitransparent beamstop

L. Porcar, D. Barkats, E. Ruiz, C. Cocho



Velocity selector

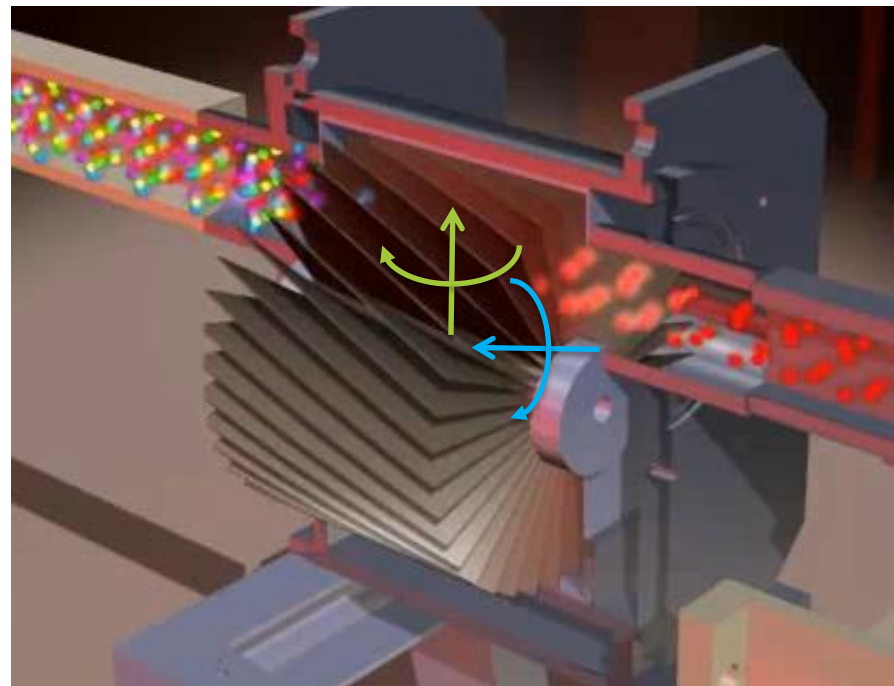
Wavelength and Smearing

Selector Speed \rightarrow Nominal Wavelength (6 - 12 Å)

Selector Tilt \rightarrow Wavelength Spread

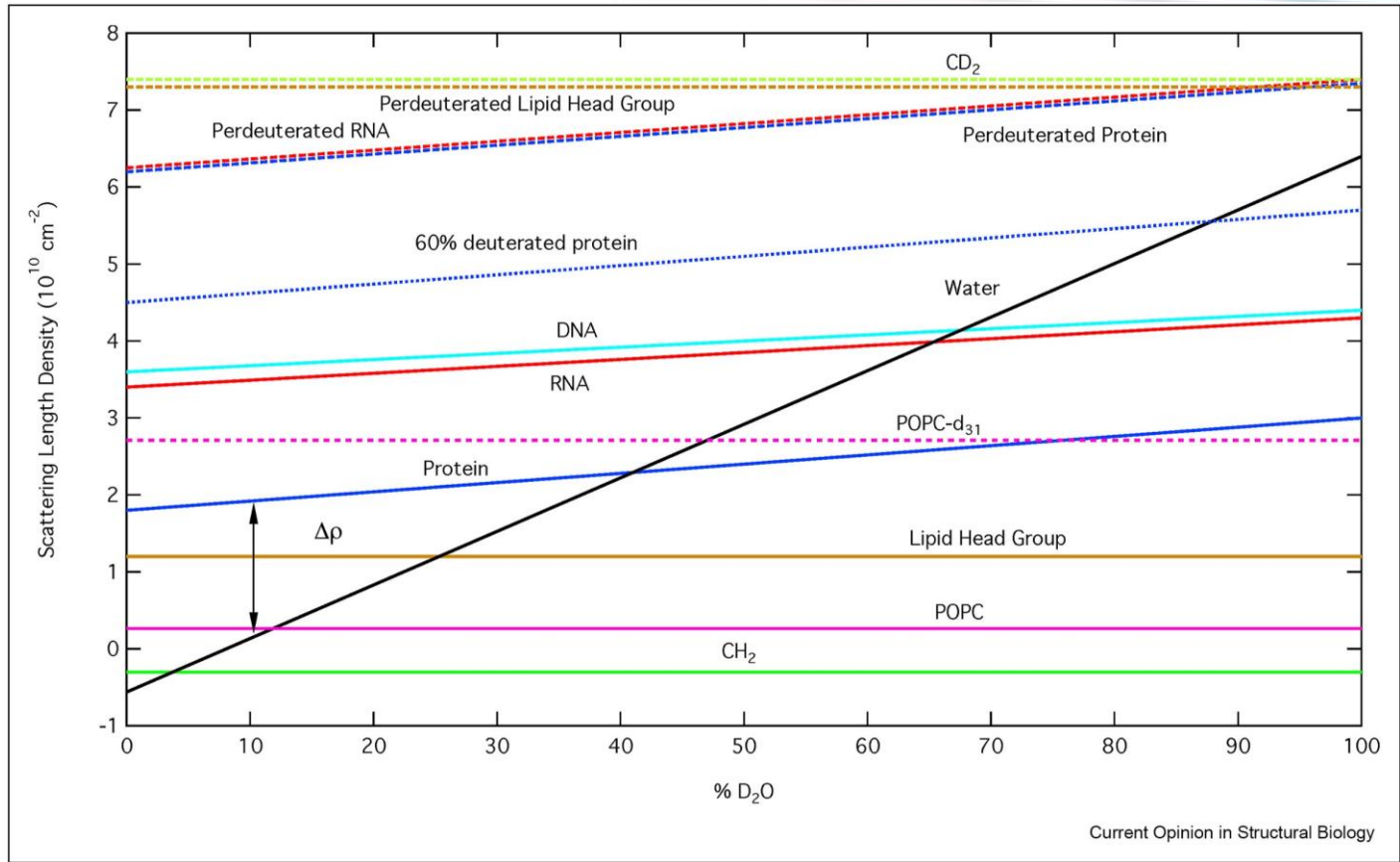
Wavelength Spread
Beam size
Sample size
pixel size

} Smearing or Q-resolution
(4th column in data files)



$$Q = 4 \pi \cdot \sin\theta / \lambda$$

Refraction based monochromators also exist for neutrons (D16). Lower flux!



Krueger 2022, <https://doi.org/10.1016/j.sbi.2022.102375>

Basic sample requirements

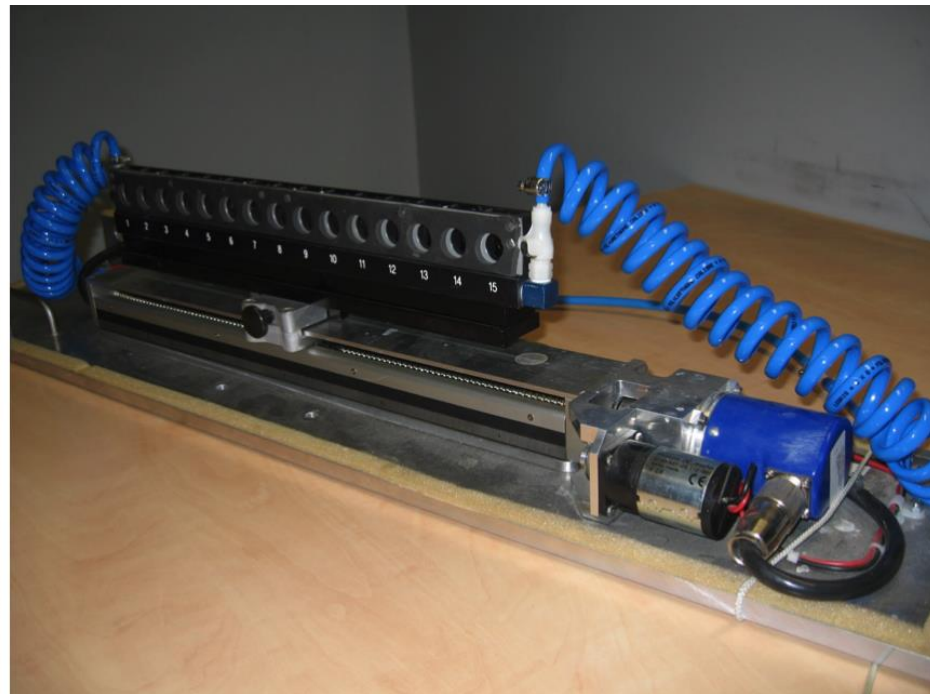
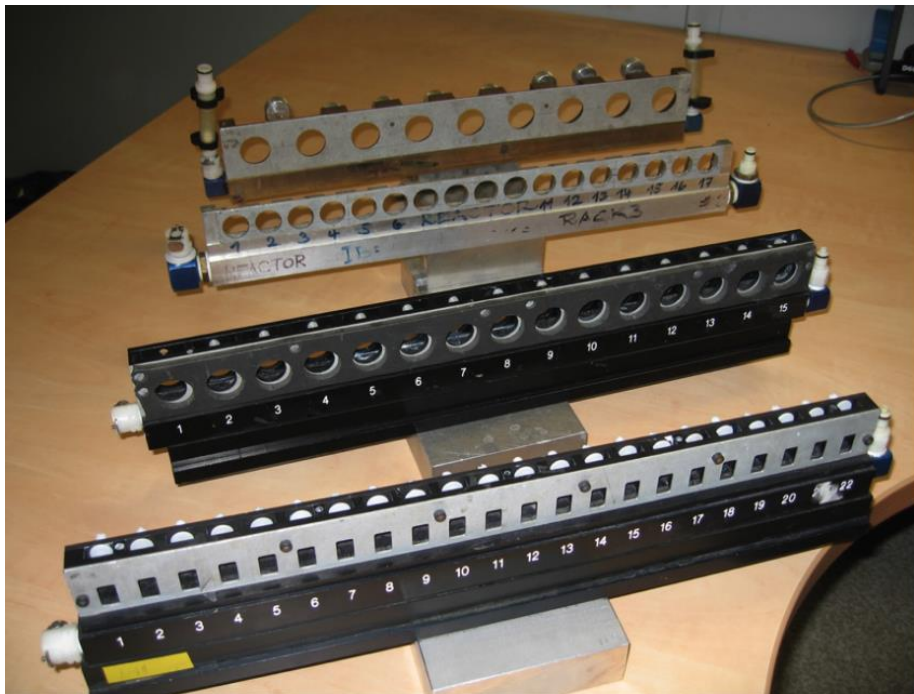
- Large enough sample quantity: one cuvette = 200uL at $C \geq 1\text{mg/mL}$ of non-matched out part of sample.
- Monodispersity and absence of interactions (according to analysis, as for SAXS)
- Optimized contrast:

Intensity proportional to contrast².

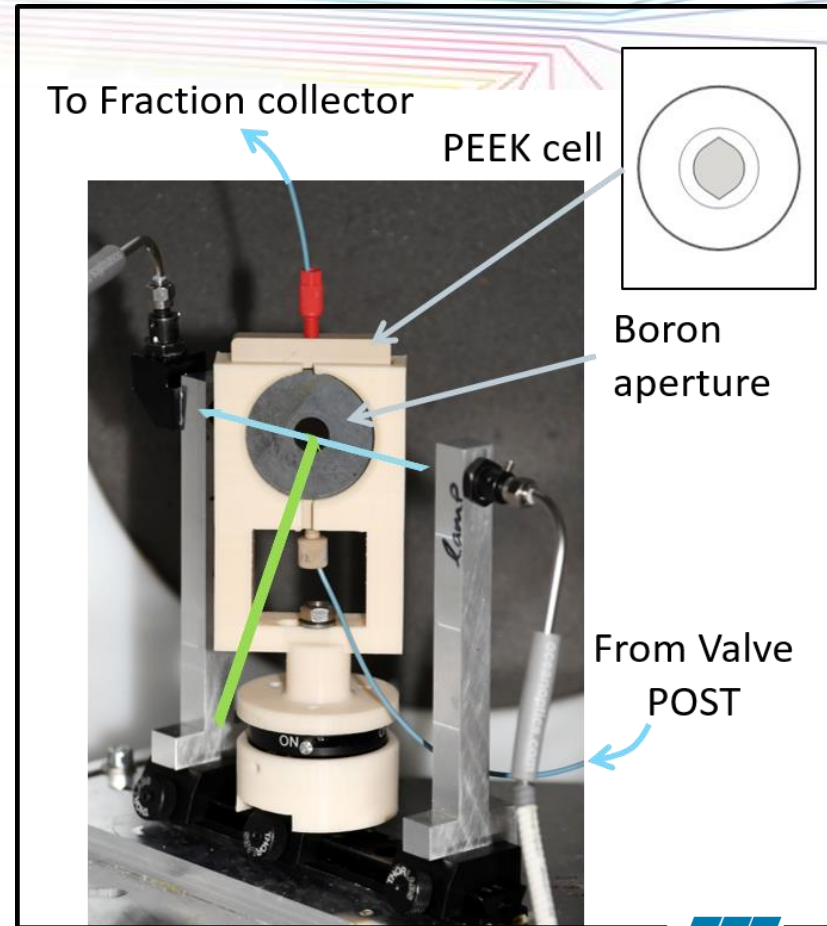
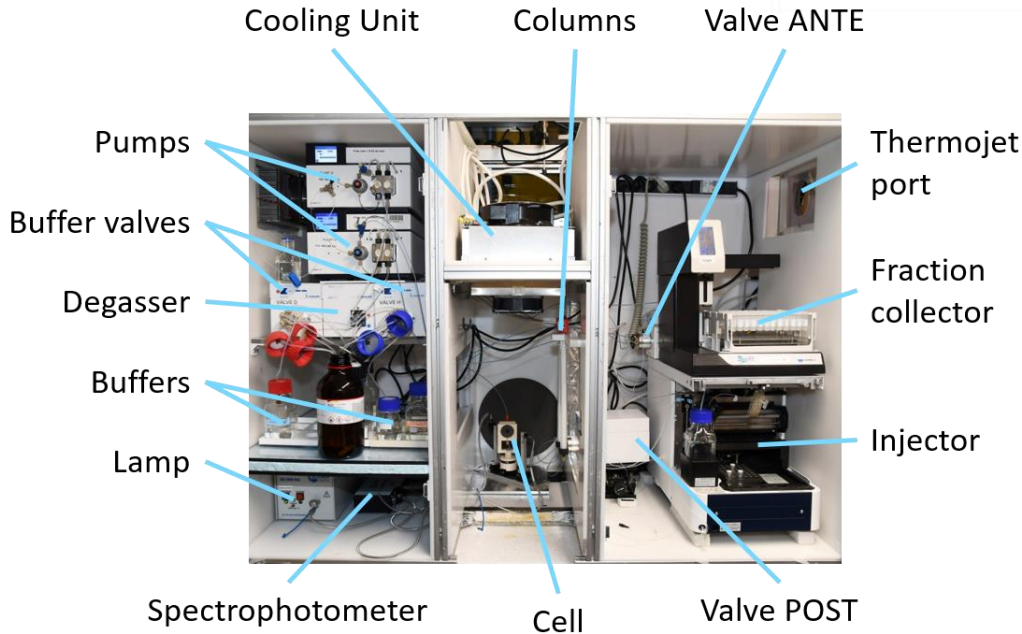
Background proportional to H₂O buffer content (from 0.05 to 1 cm⁻¹).

>> The ideal sample is an hydrogenated molecule in D₂O buffer. Matched out partners should be deuterated to have the same SLD as D₂O.

Sample changers



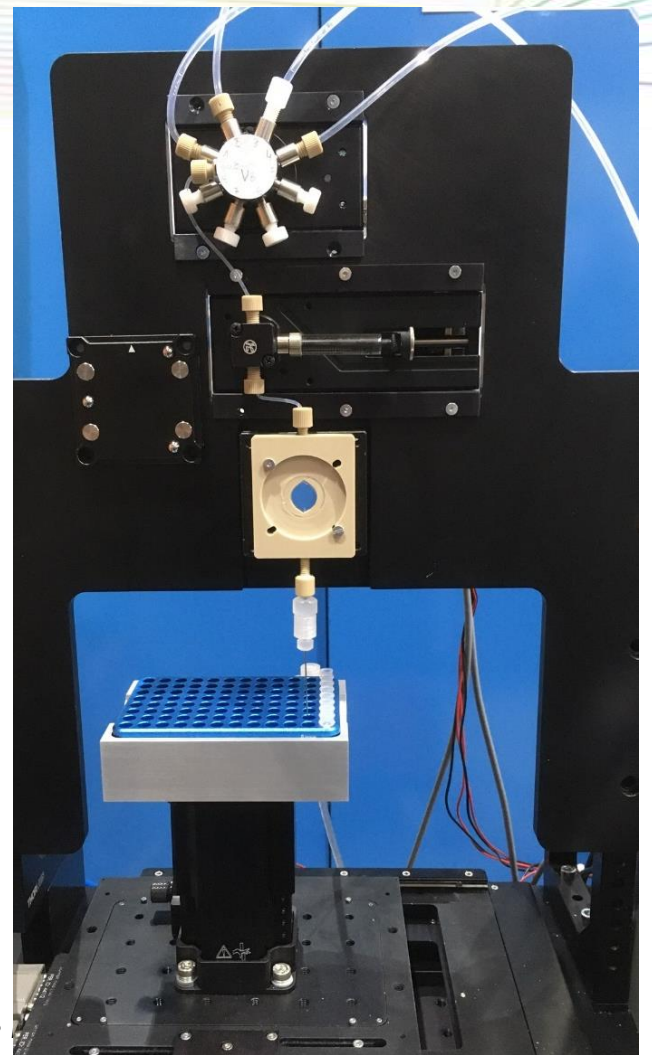
SEC-SANS



Buffer and protein measured in the same cell
> improved buffer subtraction

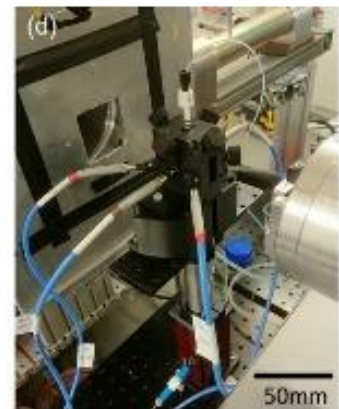
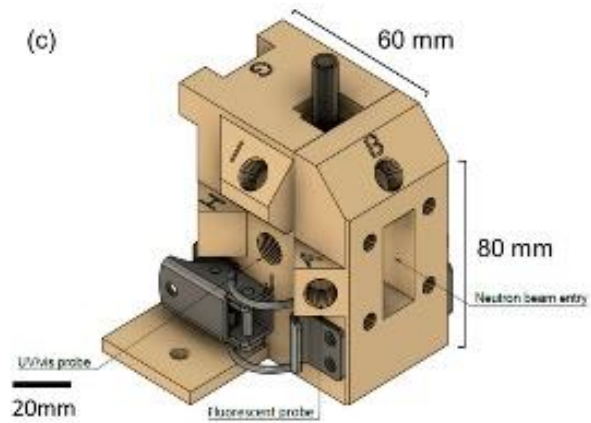
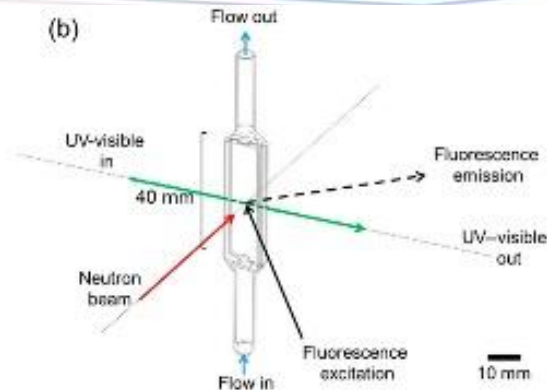
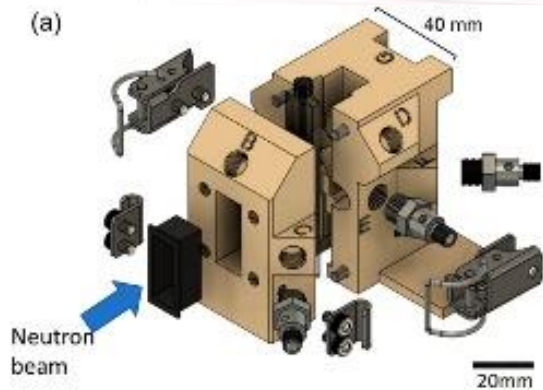
Autosampler

- Up to 96 samples, in PCR tube strips (like SAXS)
- Volume 200uL
- Up to 8 cleaning/rinsing/drying fluids
- Temperature controlled by thermojet



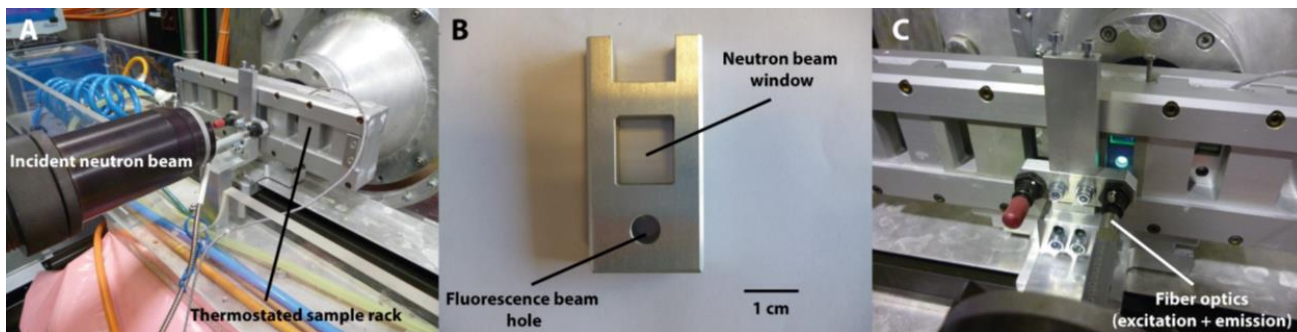
NURF

NURF—Optimization of *in situ* UV-vis and fluorescence and autonomous characterization techniques with small-angle neutron scattering instrumentation [C. Dicko](#) et al., Review of Scientific Instruments **91**, 075111 (2020)

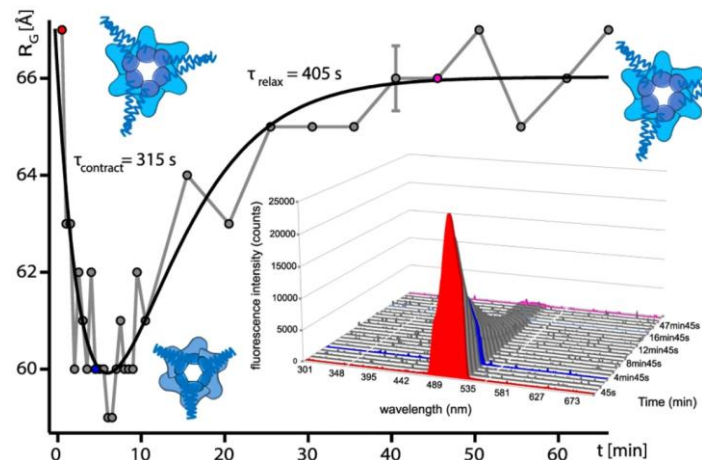


cedric.dicko@tbiokem.lth.se

In situ Fluo



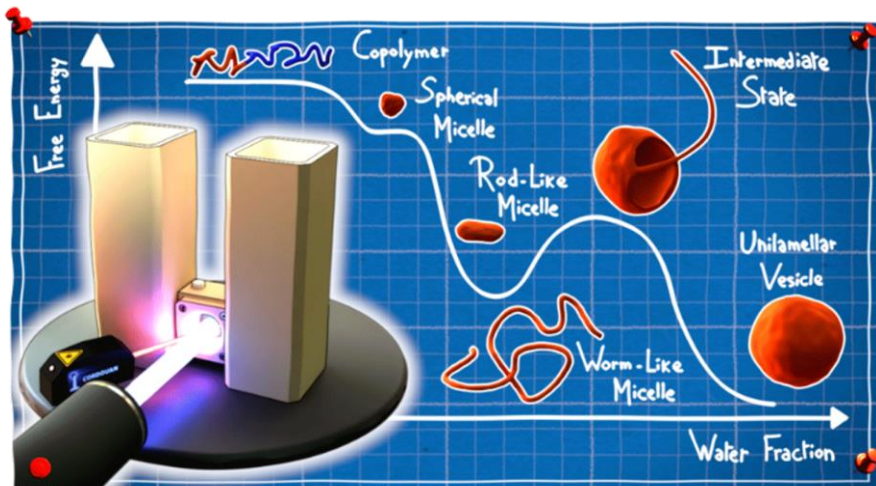
Ibrahim Z. *et al.* Time-resolved neutron scattering provides new insight into protein substrate processing by a AAA+ unfoldase. *Sci Rep* **7**, 40948 (2017).



Dialysis Cell

In situ monitoring of block copolymer self-assembly via solvent ex-change through controlled dialysis with light and neutron scattering detection

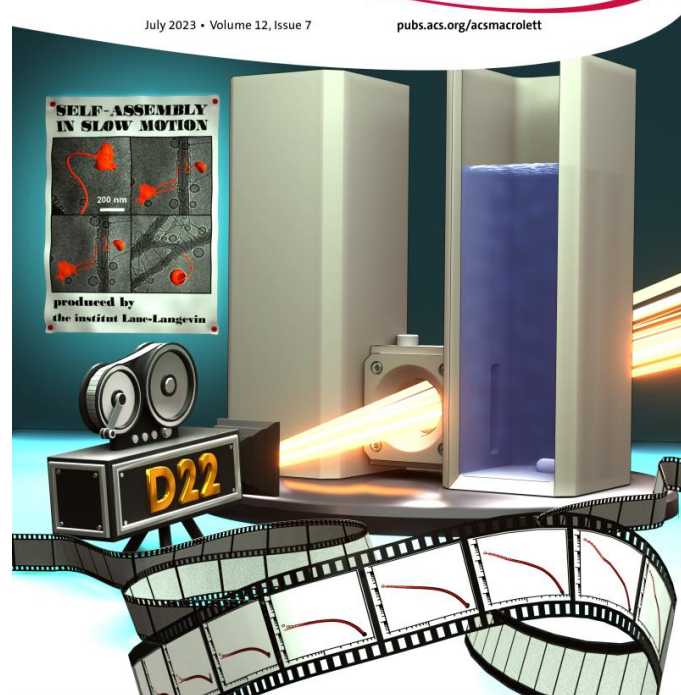
Martin Fauquignon,* Lionel Porcar,* Annie Brûlet, Jean-François Le Meins, Olivier Sandre, Jean-Paul Chapel, Marc Schmutz, and Christophe Schatz*



ACS **Macro Letters**

July 2023 • Volume 12, Issue 7

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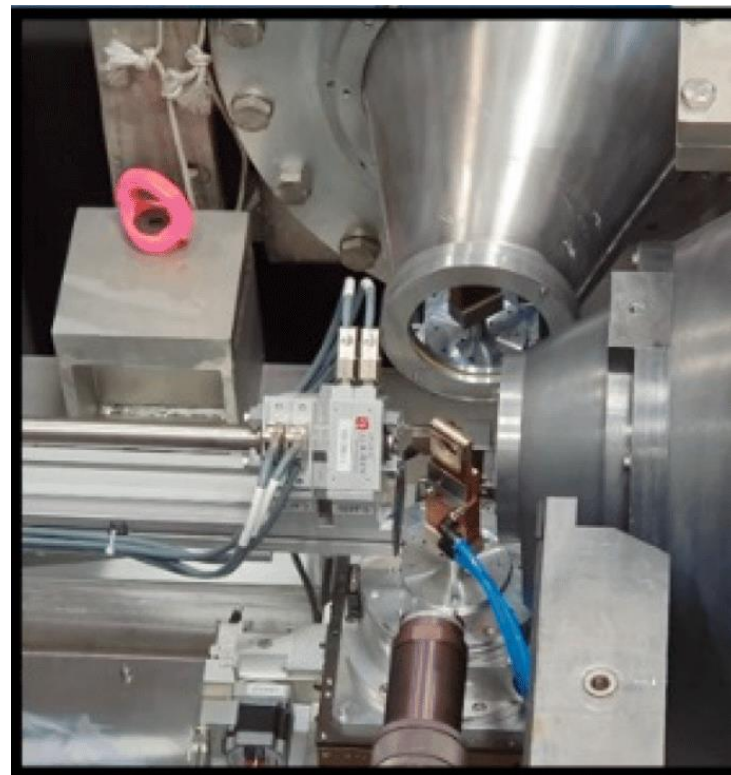
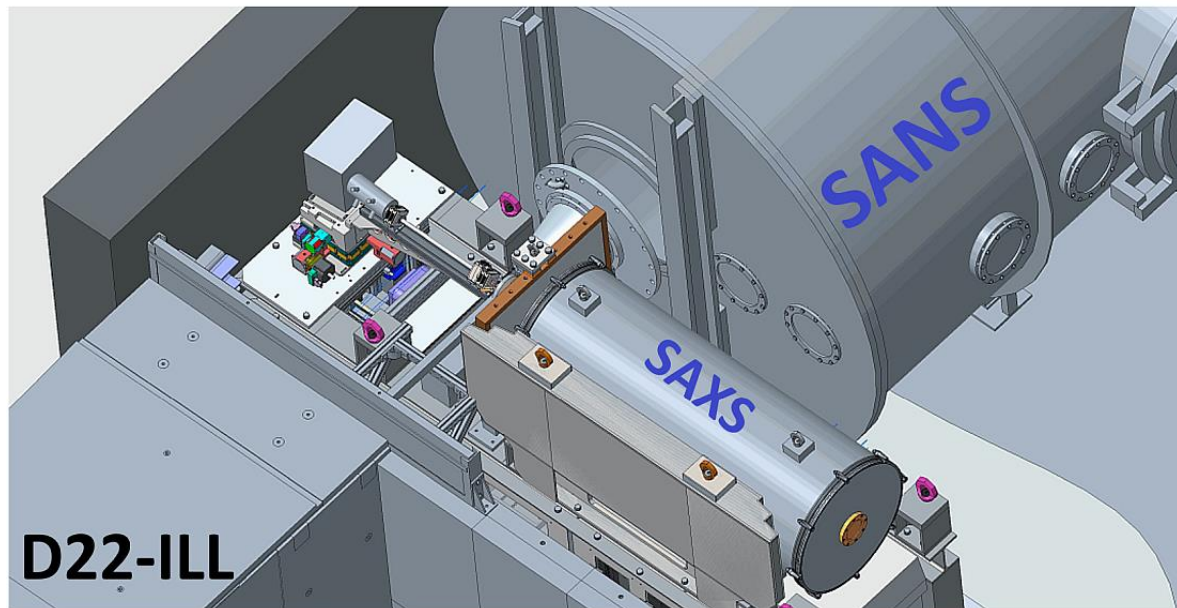
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SAXS-SANS

Simultaneous SAXS/SANS Method at D22 of ILL: Instrument Upgrade

Ezzeldin Metwalli, Klaus Götz, Tobias Zech, Christian Bär, Isabel Schuldes,
Anne Martel, Lionel Porcar and Tobias Unruh





For biologists: SAXS-SANS platform

ESRF/BM29 and ILL/D22-D11-D33

Sample requirements for SAXS, for SANS

Beamtime application at ILL

Compared to SAXS

Clear weaknesses:

- Low flux: big samples, long measurement times (stability, time resolution)
- Broad wavelength: resolution smearing along Q
- Potential sample activation

But, a few advantages:

- No radiation damage
- Contrast variation
- Large air gap to accommodate sample environment

Thank you!

Questions, Suggestions...?

