

SANS: practical aspects

Anne MARTEL, D22, LSS group

1-Jul-22

Anne Martel

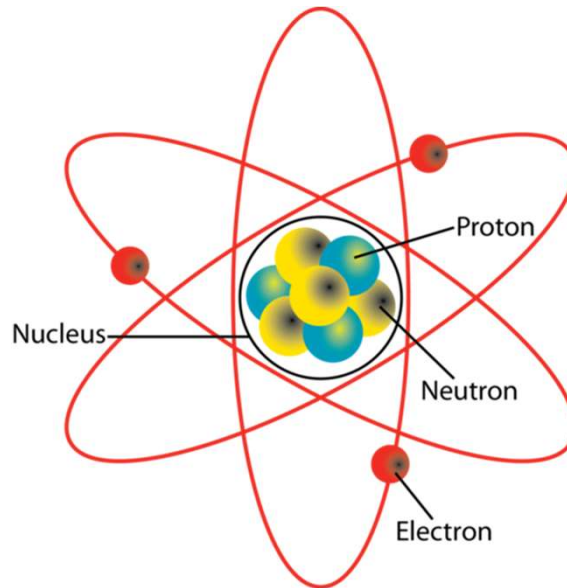
martela@ill.fr

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Introduction:

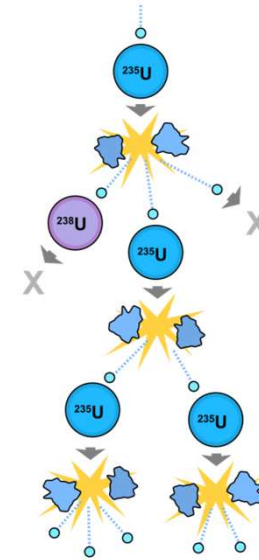
Neutrons:

Neutrons are part of the nucleus of any atom.

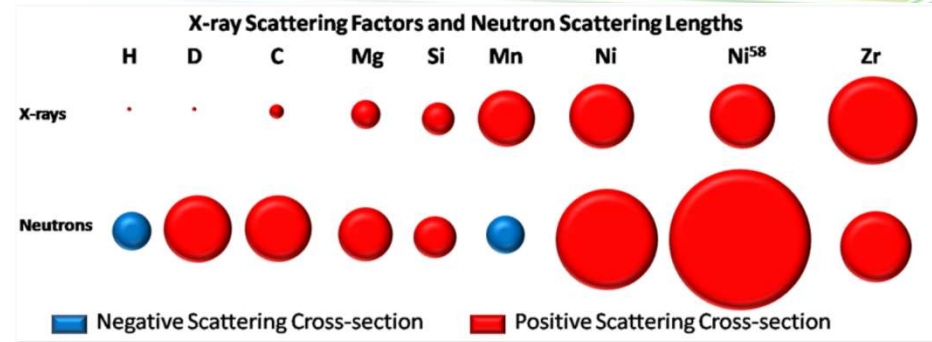


Main strength: Neutrons “see” hydrogens.

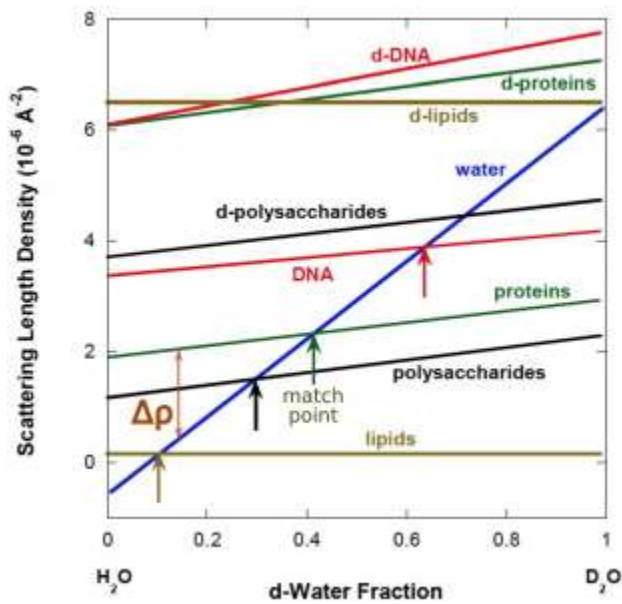
ILL, the European neutron source, produces neutrons by nuclear reaction



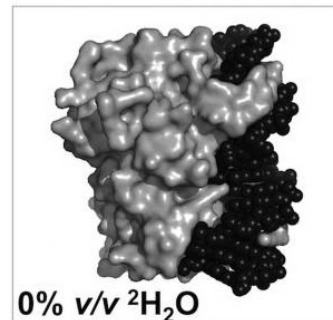
Neutrons vs X-rays: Contrast Variation



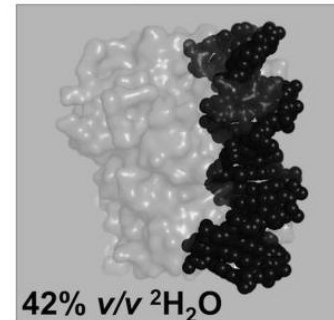
<http://www.ncnr.nist.gov/resources/n-lengths/>
http://www.isis.rl.ac.uk/ISISPublic/reference/Xray_scalfac.htm



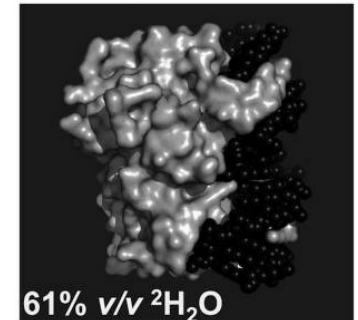
**Protein/DNA
Complex**



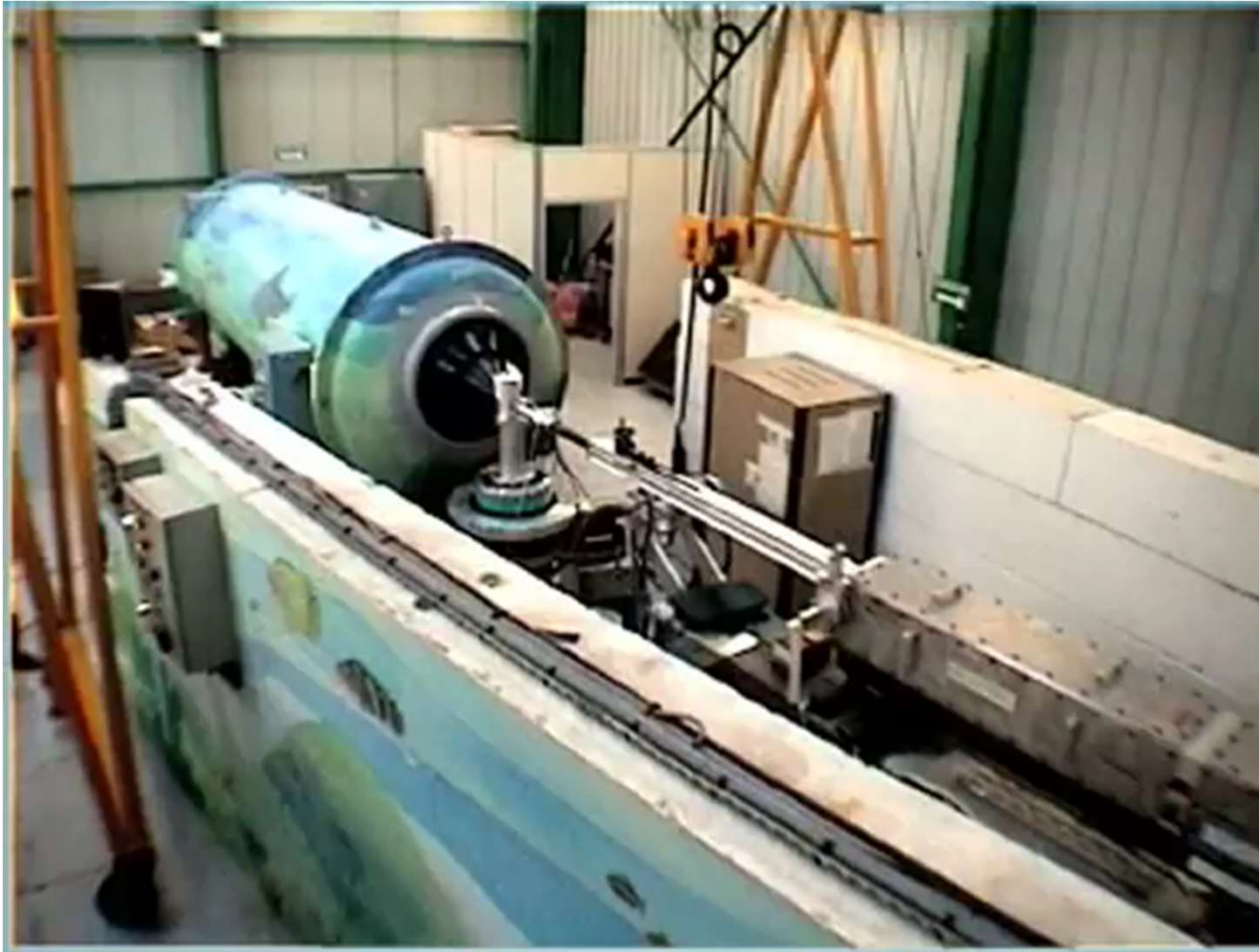
**Protein match
point**



**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

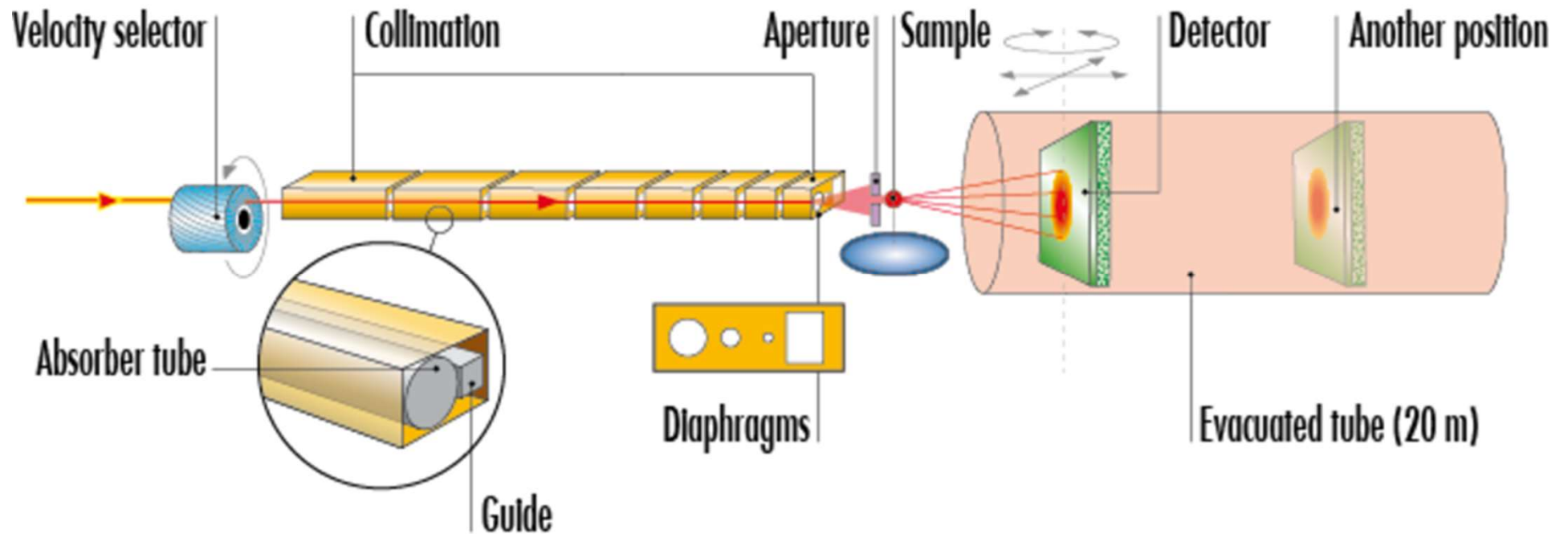
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D22, a monochromatic SANS instrument



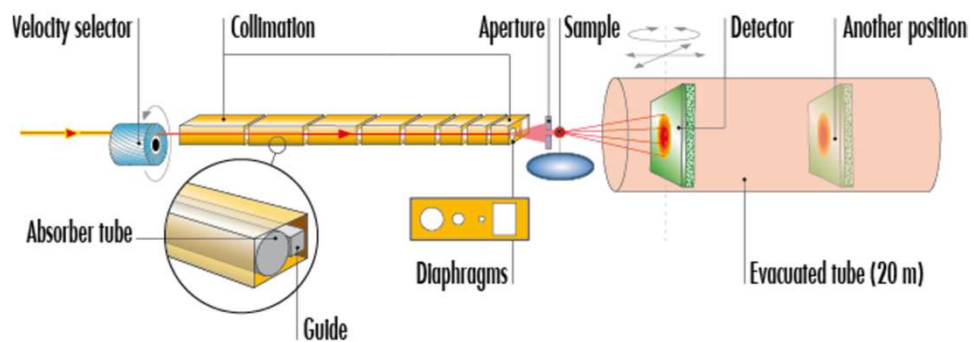


D11 description:

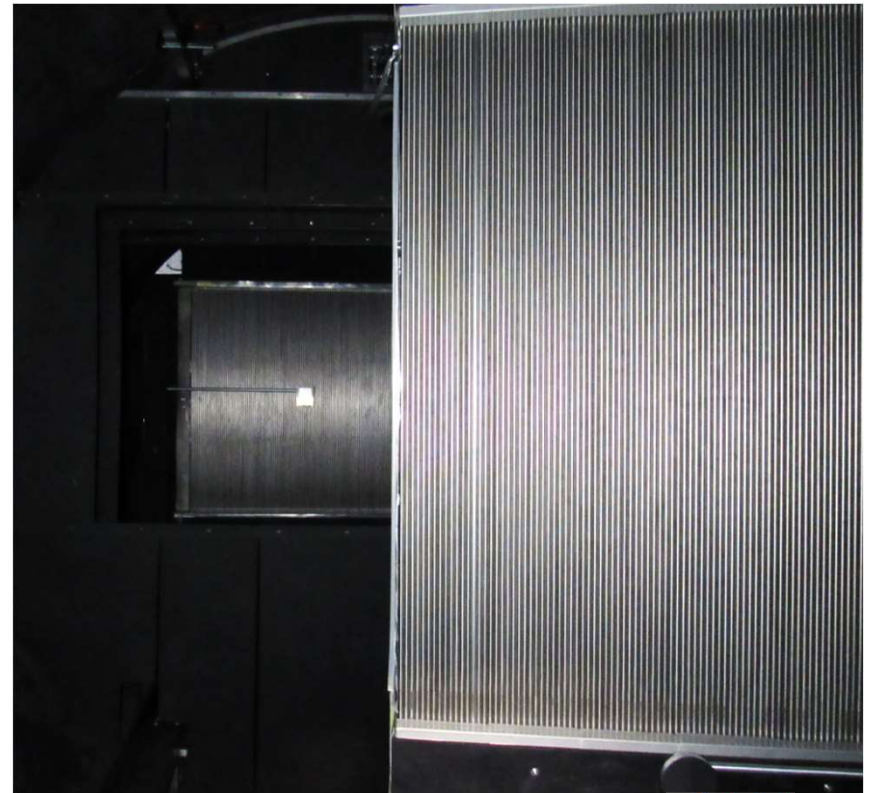
https://www.ill.eu/fileadmin/user_upload/ILL/3_Users/Instruments/Instruments_list/00_-_LARGE_SCALE_STRUCTURES/D11/html5/D11-principle/D11.html

A. Filhol

D22 ++



2nd detector > whole Q-range in one set up
 L. Porcar, R. Barkats, E. Ruiz, C. Cocho



Velocity selector

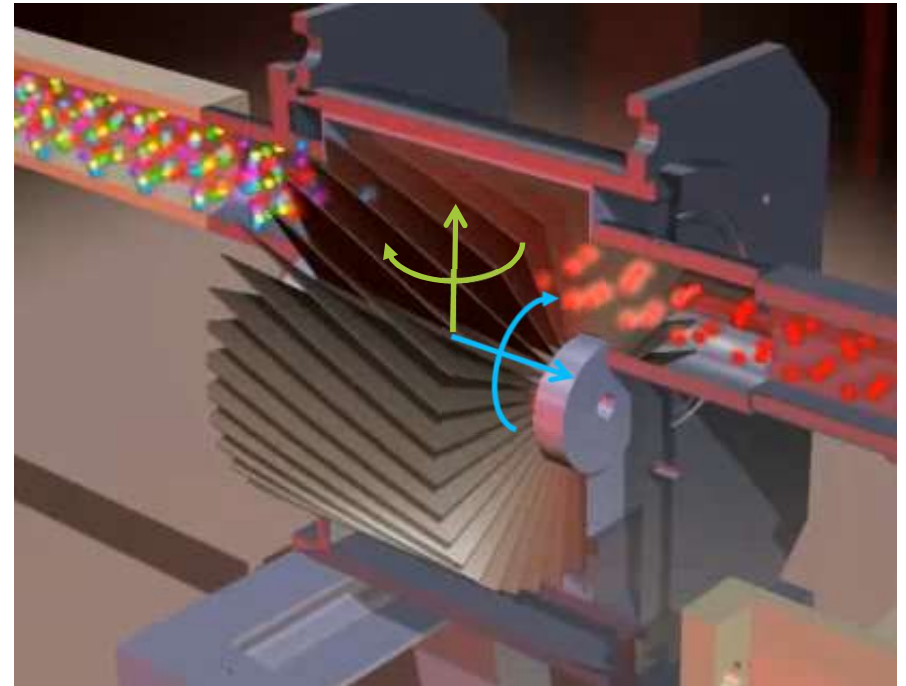
Wavelength and Smearing

Selector Speed → Nominal Wavelength (6 - 12 Å)

Selector Tilt → Wavelength Spread

Wavelength Spread
Beam size
Sample size
pixel size

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



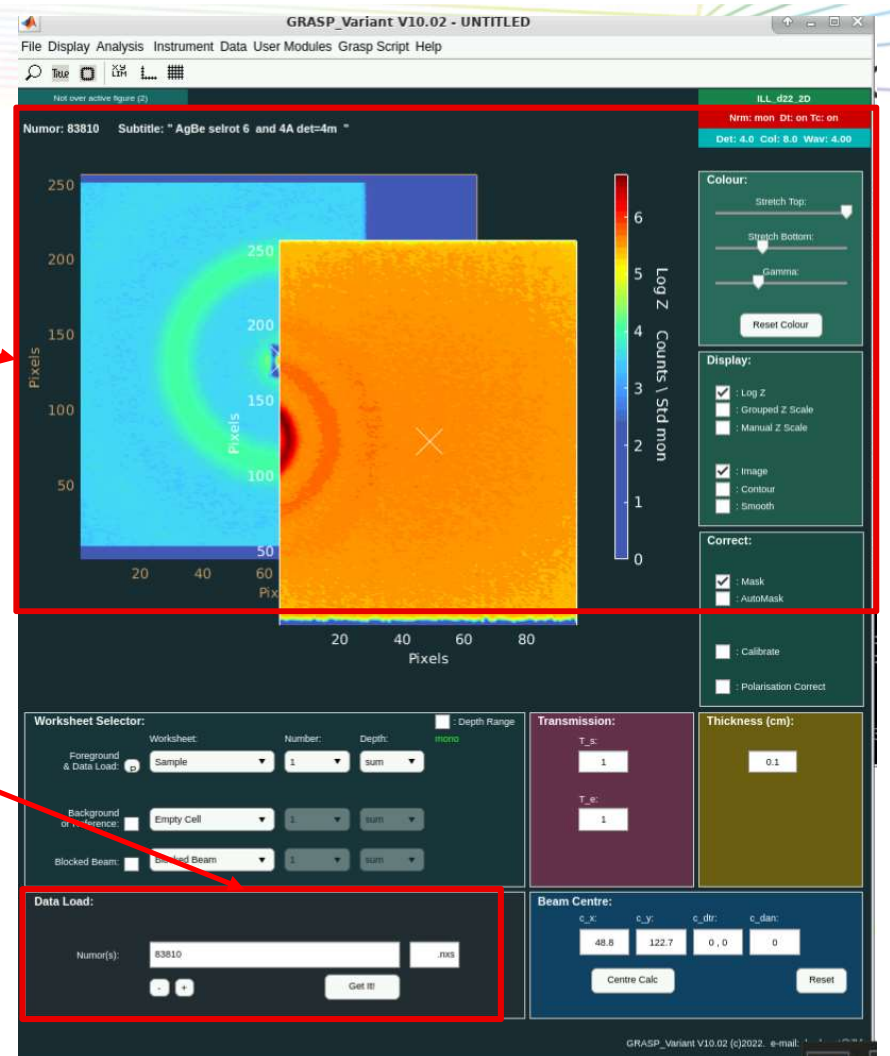
$$Q = 4 \pi \cdot \sin\theta / \lambda$$

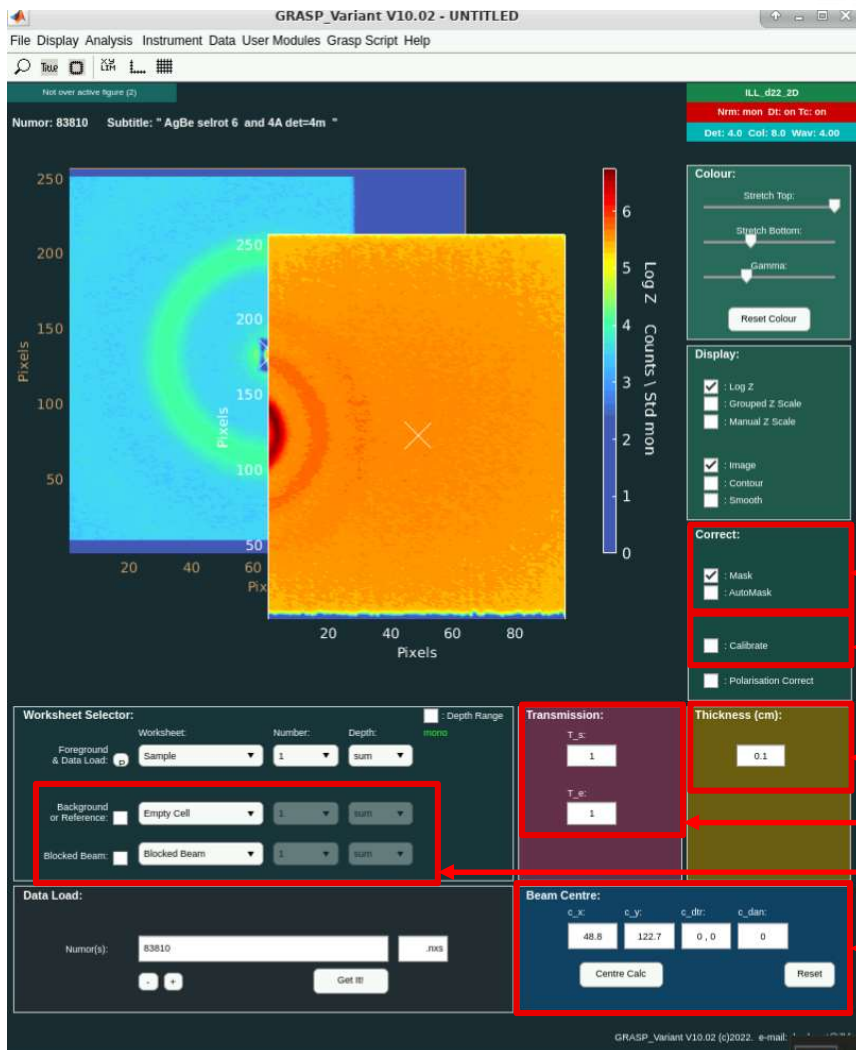
Data Reduction:

Using Grasp, on Visa

Data visualisation

Data files loading





Corrections settled
by the local contact

Mask definition

Absolute Intensity Calibration

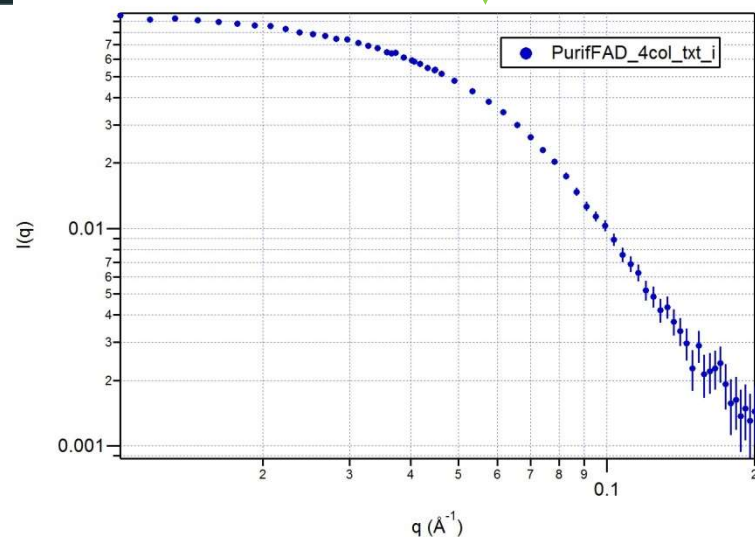
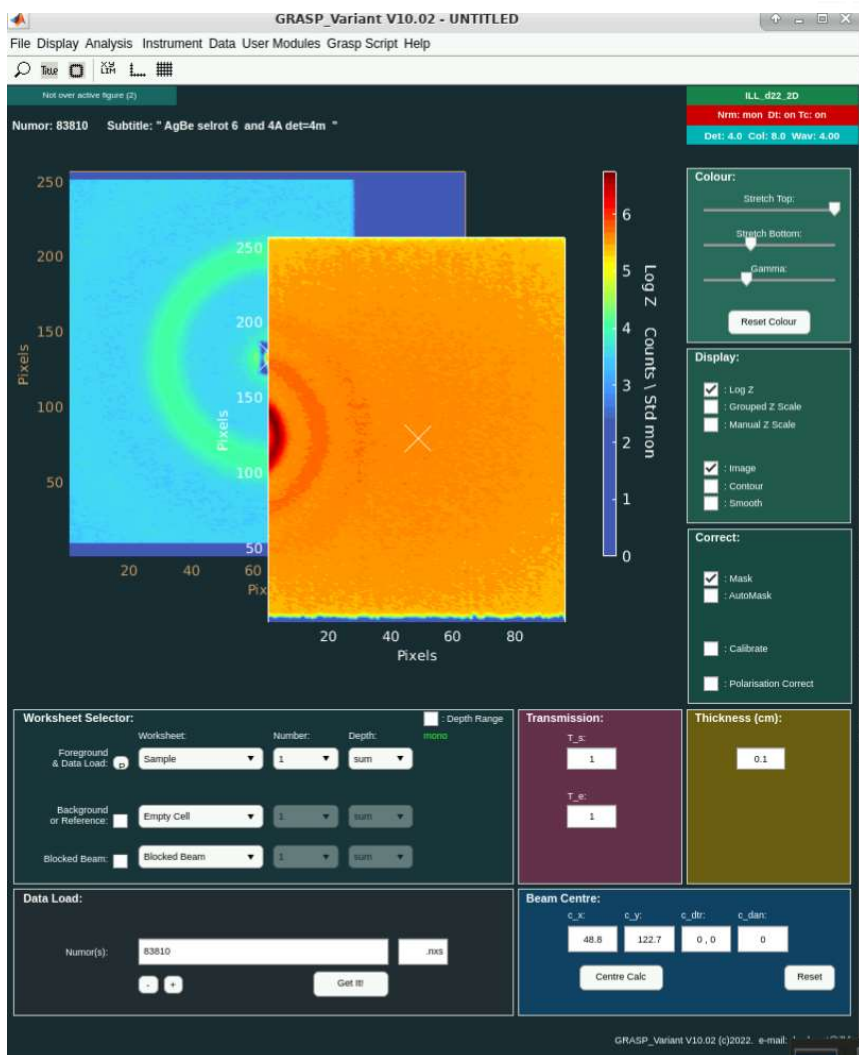
Sample Thickness Normalisation

Transmission Normalisation

Empty Cell and Blocked Beam subtraction

Beam center on both detectors

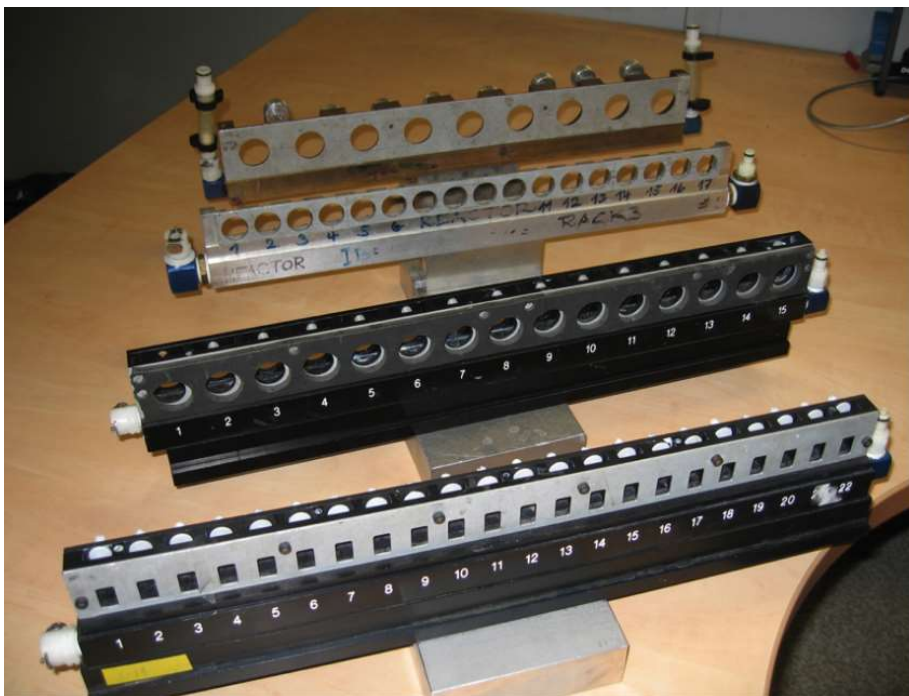
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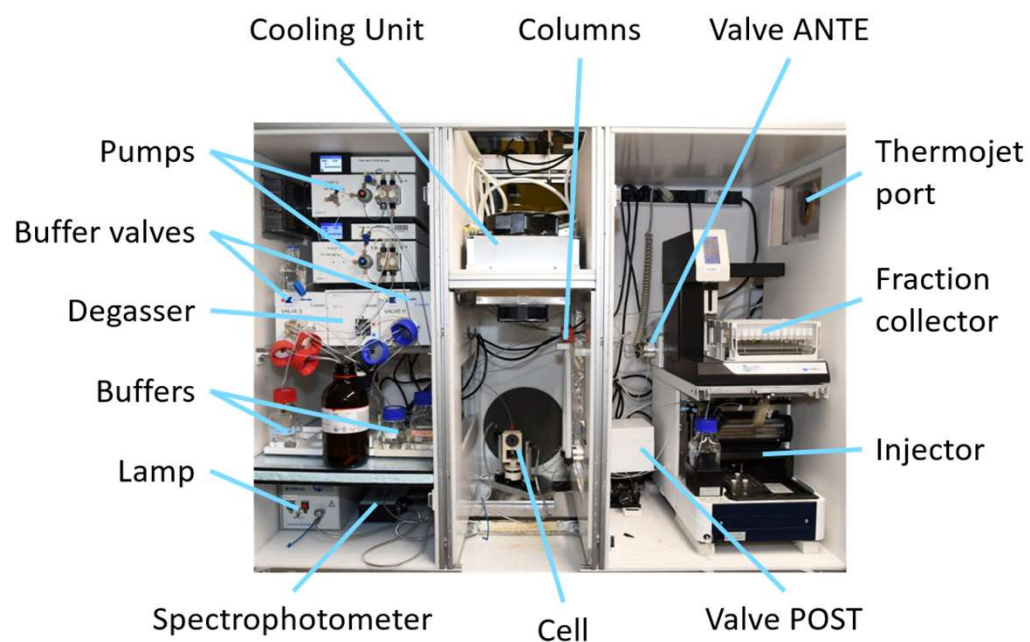
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Sample environment:

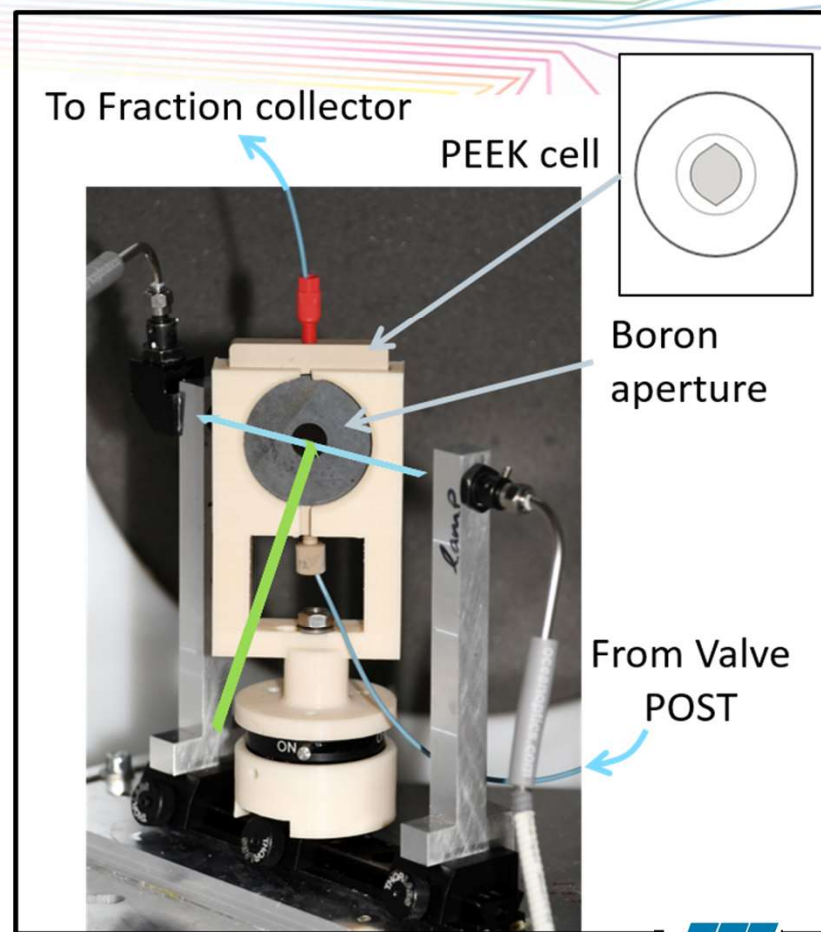
Sample changers (200uL or 300uL)

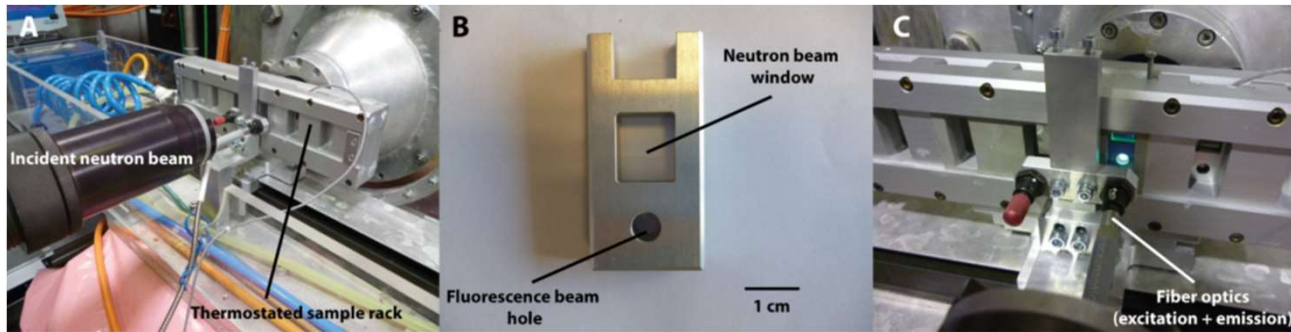


In situ SEC

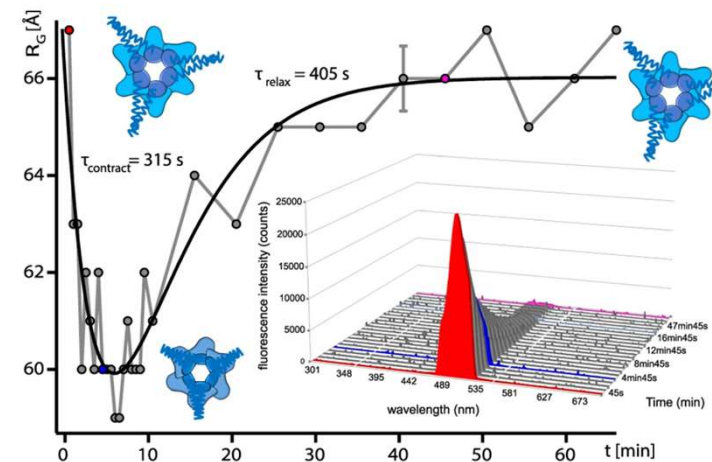


Buffer and protein measured in the same cell
> improved buffer subtraction





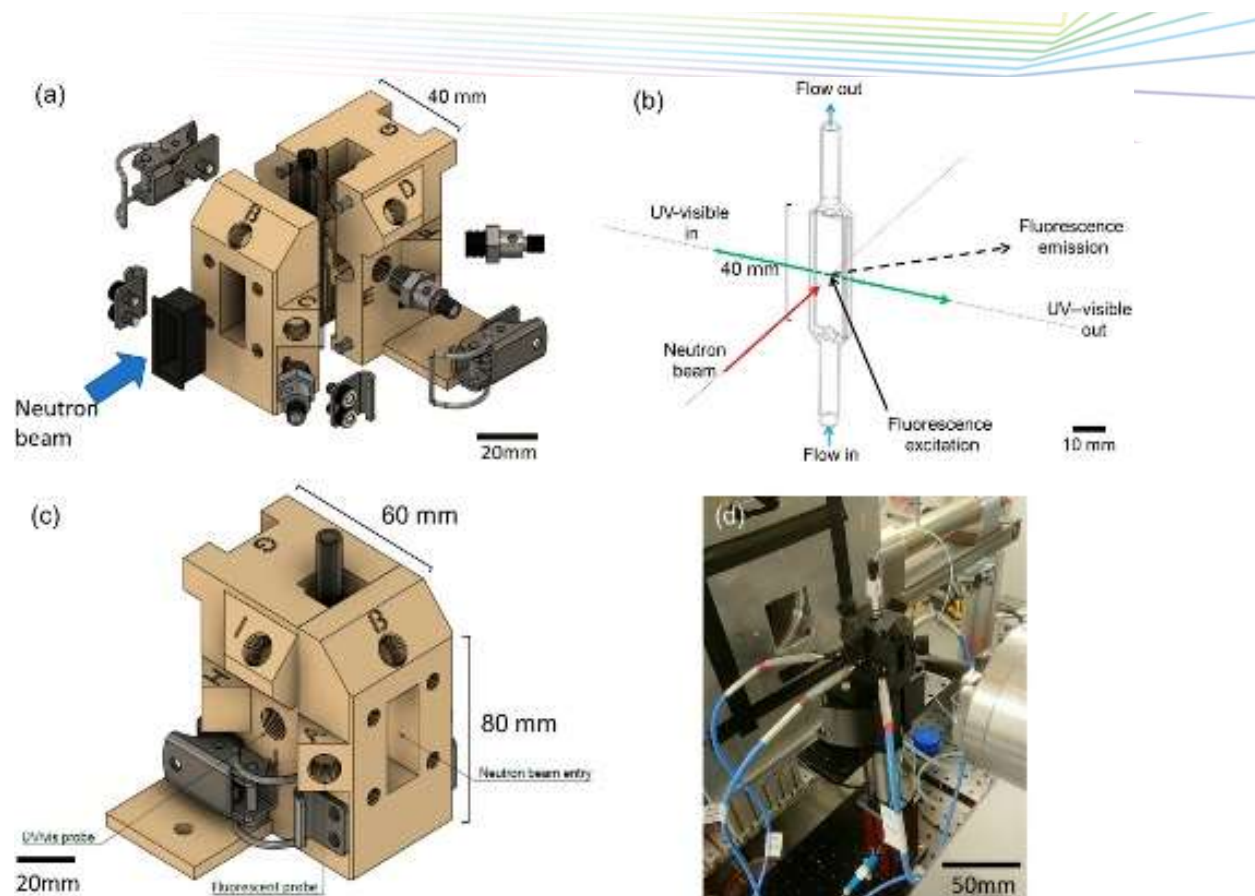
Ibrahim Z. *et al.* Time-resolved neutron scattering provides new insight into protein substrate processing by a AAA+ unfoldase. *Sci Rep* **7**, 40948 (2017).



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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)



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Autosampler

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





Thank you!

Questions, Suggestions...?