Solution scattering from biological macromolecules
19 – 26 November 2018 | Hamburg, Germany

26 course participants
(19 nationalities representing institutes from 17 countries)

1 local attendant

9 external lecturers and 9 tutors/lecturers from EMBL-Hamburg
EMBL Outstation at DESY, Hamburg

1974

44 years later

EMBL synchrotron facilities at the upgraded Petra-3 ring

- 2 MX beamlines (P13, P14)
- 1 BioSAXS beamline (P12)
- Sample preparation and characterization facility (SPC)

EMBL-Paradise
Group leader: D. Svergun


Postdocs: M. Schroer, A. Gruzinov, S. da Vela, D. Molodenskiy, N. Hajizadeh

Predocs: K. Malanastas, T. Cheremnykh

Major tasks:

- Development of data analysis methods
- Running and developing SAXS beamlines
- User support and collaborative projects
- Interactions, education and training
Small-angle scattering in structural biology

In preparation for an EMBO Course … (courtesy of F.Gabel, IBS, Grenoble)

The new SAS book is not yet available for everyone (courtesy of M.Graewert, EMBL-HH)

Data analysis

Flexible systems

Bioinformatics
Biochemistry
AUC
FRET
EPR

Scattering curve

Radiation sources:
- X-ray tube (λ = 0.1 - 0.2 nm)
- Synchrotron (λ = 0.05 - 0.5 nm)
- Thermal neutrons (λ = 0.1 - 1 nm)

Sample
Solvent
Incident beam
Wave vector k, k = 2π/λ
Detector
Scattered beam, k1

EPR

Small-angle scattering in structural biology

Resolution, nm:
- 3.1
- 1.6
- 1.0
- 0.8

MS

Distances

Additional information

2θ

Sample

1

2

3

4

5

6

7

8

lg I, relative

Resolution, nm:
- 3.1
- 1.6
- 1.0
- 0.8

In preparation for an EMBO Course … (courtesy of F.Gabel, IBS, Grenoble)

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On finishing my university studies, in 1936, I obtained a post as assistant, which gave me the opportunity to work towards my thesis…

My “boss”, who looked after my dissertation, … was a crystallographer who kept an eye on my work rather distantly, but he did pass on a very good idea on me: to study, in addition to Bragg diffractions, diffuse scattering.

<He> asked me to make a camera with monochromatic primary radiation and with minimum parasitic radiation… That is why I studied especially small-angle scattering. I observed that … the scattering is strong when the sample contains fine grains (10 to 100 nm).

I produced next the means of determining the grain size from the scattering curve. It was the beginning of X-rays small-angle scattering…

When biologists go for SAS

This is just a trivial case:
You will learn that SAXSMAN (© A.Kikhney) yields much more

Care for a shape?
High brilliance EMBL SAXS beamline P12

- About $10^{13}$ ph/sec in 200*120 mm$^2$
- Energy between 4 and 20 keV (3.0 to 0.6 Å)
- Divergence below 0.05*0.05 mrad$^2$
- Multilayer monochromator mode: over $5 \times 10^{14}$ ph/sec
- SASFLOW pipeline for on-line data processing and analysis
- Full automation, remote and mail-in access

- Robotic EMBL/ESRF sample changer
- Automated FPLC/HPLC in parallel with biophysical sample characterisation
ATSAS (All That SAS) roadmap

- World most comprehensive program suite for small-angle scattering data analysis from biomacromolecular solutions
- Consists of more than 80 programs developed at EMBL-HH since 1991
- Available for download since 1999, accessible online since 2006
- Presently, ATSAS has over 16,000 users from over 50 countries; online usage: over 4,000 users/~35,000 jobs per year
Schedule of the Course

- Day 1: Basics of small-angle scattering (Mon 19 Nov)
- Day 2: From sample to data (Tue 20 Nov)
- Day 3: From data to shape (Wed 21 Nov)
- Day 4: Rigid body (hybrid) modelling (Thu 22 Nov)
- Day 5: Mixtures and interacting systems (Fri 23 Nov)
- Day 6: SAXS and complementary methods I (Sat 24 Nov)
- Day 7: SAXS and complementary methods II (Sun 25 Nov)
- Day 8: General discussion (Mon 26 Nov)
Lectures and Practicals

- **Theory Lectures** (48e Seminar Room, 2nd floor)
- **Software Demonstrations/Tutorials** (48e Seminar Room, PC, LCD projector)
- **Structural Biology Seminars** (48e Seminar Room, 2nd floor)
- **Practicals:** (P12 beamline and user room, 48e, ground floor).
- **Data Analysis and SAXS Quest** (48e Seminar Room, 2nd floor)
SAXS Play Station VI (anti-sleeping pills)

- SAXS Quest
Practical measurements at P12

- **Own samples**
  - Those who brought their own samples, shall measure them, analyse the data, and report the results at the end of the Course.

- **No own samples**
  - Those who brought no samples, shall measure the alien proteins provided by us, analyse the data, and report the results at the end of the Course.

- **Measurements on Mon 19.11 and Tue 20.11**
  - Sample changer+SEC-SAXS setup

- **Measurements on Fri 23.11**
  - Sample changer
Whom to ask

- **General questions:**
  - Dmitri Svergun (internal 125, mobile *127), Alexey Kikhney (170, mobile *150)

- **Organizational questions:**
  - Margret Fischer (internal 110, mobile *108)
  - Sarah Marshall (111)

- **Computer hardware:** Felipo Goncalves (133)

- **Computer software:**
  - Daniel Franke (244), Nelly Hajizadeh (217), Peter Konarev (129), Maxim Petoukhov (179)

- **SAXS practicals:** Clement Blanchet (192), Martin Schroer (241), Melissa Graewert (115), Cy Jeffries (177)

- **Beamline P12 phone:**
  - 040 89902 312 (internal 312)
Miscellaneous

- **Course photos:** 20.11 and 24.11, first coffee breaks
- **Free afternoon:** Thursday, 22 November
- **Course dinner:** Sunday November 25, as of 20:00
- **Pairing for the Quest:**
  - The list is given in the Course materials
  - Quest winners will get very SAXSy prizes
  - Quest run starts tomorrow
- **Own laptops:** network 'EMBL_GUEST' (password available in the seminar room)
- **Your presentations:**
  - 26 participants (with or without PPT, as you wish)
  - Will be on the 1st and 3rd days (19.11 + 21.11)
  - 8 minutes per participant (SHARP: 6 min talk + 2 min questions)