The Compact Solution for High-Throughput Nanostructure Analysis

Anton Paar

SAXSpace

SAXSpace: The reliable partner for routine SAXS and WAXS analysis

The SAXSpace system for the lab is the workhorse for routine analysis of multiple samples, in particular biological samples (BioSAXS), surfactants, and nanoparticle dispersions. Combined with state-of-the-art software and data analysis, SAXSpace ensures fast and straightforward investigations of multiple nanostructured samples.

More than 60 years of SAXS expertise are the basis for a versatile instrument built for high-throughput routine measurements and fast analysis of your nanostructured materials.

Brilliance your way

SAXSpace is a robust lab-scale SAXS/WAXS system meeting the highest demands:

- Excellent resolution at a compact size: q_{min}: 0.03 nm^{-1}
- Short measurement time and the highest SAXS/WAXS data quality
- High sample throughput: up to 192 liquid samples
- High system uptime and easy operation

60 years of innovation in SAXS

1957
First commercial SAXS analyzer by Otto Kratky, built by Anton Paar

1981
Kratky Compact Camera

2003
SAXSess

YOUR RELIABLE PARTNER FOR

SAXSpace

NANO RESEARCH IN THE LAB

2012
SAXSpace

2015
SAXSpoint

2017
SAXSpoint 2.0

Features

Powerful X-rays – fast results

SAXSpace employs the powerful Primux 3000 X-ray source by Anton Paar together with customized optics by AXO Dresden. This combination ensures a highly intense and monochromatic X-ray beam.
The well-proven scatterless block collimation concept, initially developed by Anton Paar together with SAXS "founding father" Otto Kratky in the 1950s, provides a well-defined and intense X-ray beam which illuminates a large sample volume. In consequence you benefit from a very short measurement time and a high signal-to-noise ratio, resulting in high-quality representative SAXS and WAXS data.

Optimized for high-throughput screening

SAXSpace is your laboratory workhorse for fast measurement and routine analysis of multiple samples. The ASX autosamplers provide fast and precise sample transport, efficient cleaning procedures, and allow you to measure up to 192 liquid samples automatically and unsupervised.
This speeds up your routine analysis, in particular of proteins in solution (BioSAXS) and nanoparticle dispersions.
Furthermore, SAXSpace features various other sample stages and holders for ambient and non-ambient SAXS and WAXS studies of many nanomaterials.

SAXS and WAXS in one go

Get all information from the same sample.
The TrueSWAXS feature collects scattering data from small to wide angles simultaneously and continuously. This unique functionality is based on precise component movements along the X-ray beam axis and therefore allows you to access a scattering angle range from the smallest angles up to 60° 2θ.
Rely on uniform resolution and reliable results without bothering about time-consuming realignment or changing the detector position.

Dedicated software

Processing and analyzing a multitude of scattering data requires optimized and powerful software packages. Make use of the user-friendly and comprehensive SAXSdrive™ and SAXSanalysis™ software packages for data acquisition as well as for data processing and analysis. Create automated serial measurements easily, including automated sampling, temperature scans, etc., and analyze large scattering data sets by using customizable templates.

Gold standard in detector technology

SAXSpace employs the latest hybrid photon counting detector (HPC) technology from Dectris. The high-resolution Mythen2 R-series and EIGER R-series detectors combine direct X-ray detection in single photon-counting mode with a small pixel size (50 µm and 75 µm), ensuring an excellent signal-to-noise ratio and the highest spatial resolution.
Both detectors are fully integrated in the SAXSpace system hardware and software so you can easily run automated SAXS and WAXS measurements in one system.

In the spotlight: BioSAXS

Structural studies of macromolecules

Small-angle X-ray scattering studies of biological materials provide unique structural information and therefore complement other techniques, such as protein crystallography, nuclear magnetic resonance (NMR), and electron microscopy (Cryo-TEM).

Challenge

Protein crystallography requires a single crystal of a biomolecule, which often is a challenge. The required "frozen", i.e. crystallized, state of a sample leaves essential questions unanswered:

- How is the sample's structure influenced by its natural environment?
- Which dynamic processes is the sample involved in?

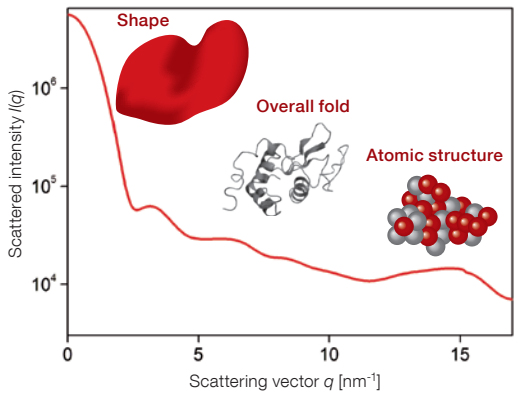
NMR and SAXS answer these questions, but while NMR delivers high-resolution structure information, its signal is often so complex that it cannot be interpreted without further input.

Solution

With SAXS, biological macromolecules and their complexes are investigated in solution, i.e. under physiological conditions. Analyzing samples in their native state is essential to study dynamic processes, such as structural changes upon ligand binding or protein folding/unfolding upon environmental changes.

Results:

- Size and shape of biological macromolecules
- 3D envelopes of proteins or protein complexes
- Degree of aggregation
- Mass analysis
- Folding and unfolding of proteins (Kratky plot)
- Protein stability upon variation of external parameters
- Structure changes due to ligand binding



Structural information of a scattering curve

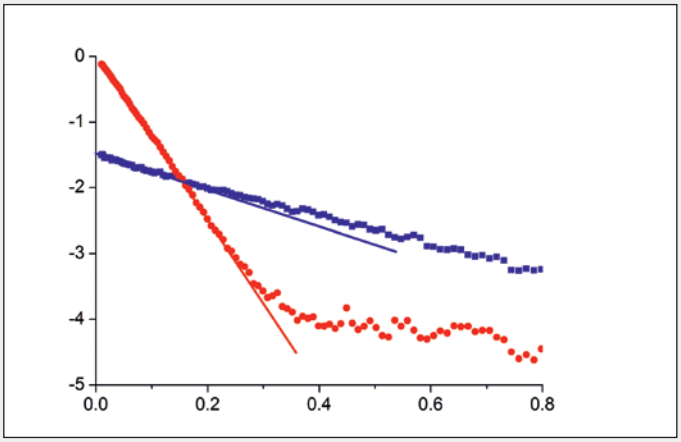
BioSAXS analysis

Determining radius of gyration, particle volume/mass and folded/unfolded status

Guinier analysis and Kratky plot

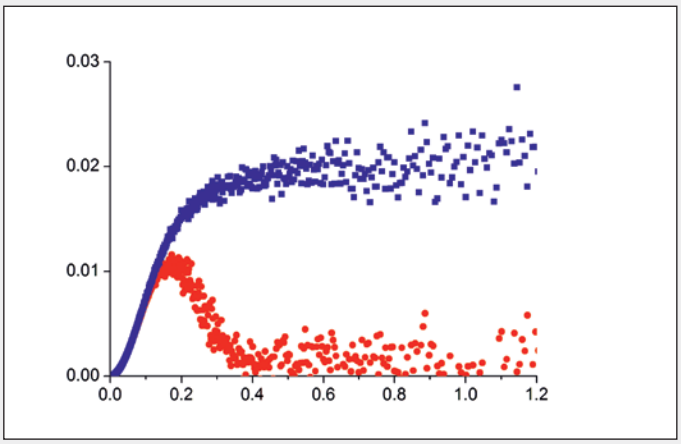
The Guinier method analyzes the scattering curve at small angles and determines two SAXS invariants:

- The radius of gyration (RG) is calculated from the initial slope and is proportional to the particle size.
- The extrapolated intensity at zero scattering angle I(0) is used to determine the particle volume which is proportional to the particle mass.



The Kratky plot provides information about protein folding and unfolding. In the I(q) q^2 vs. q (Kratky) plot

- the signal of an unfolded protein runs into a plateau
- a folded, i.e. compact, protein exhibits a distinct maximum.



Calculating 3-dimensional envelopes, particles' size, shape, and internal structure

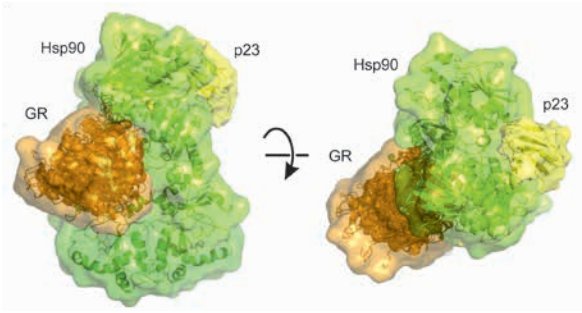
Fourier transformation

The Fourier transformation of SAXS curves uncovers information in real space and gives you access to the Pair Distance Distribution Function which allows you to extract valuable information about the particles' size, shape, and internal structure.
Based on experimental small-angle scattering data of randomly ordered dispersed particles, 3-dimensional low-resolution shapes can be calculated by using ab-initio methods. These "envelopes" visualize the protein shape and the folding of the protein backbones.

Lysozyme 3D envelope, calculated with DAMMIF[1]

Model the structure of complex assemblies

Information obtained by other techniques (e.g. protein crystallography) can be combined with SAXS data to determine the relative orientation and placement of individual domains in a complex.
This process is known as rigid body modeling. It enables you to find structures of complexes that best fit your experimental data. For example, the structure of a protein complex can be solved with the aid of the constituting proteins' crystal structure.



CORAL[2] rigid body model of the Hsp90-GR-p23 complex[3]

Application fields

- Biological samples (BioSAXS)
- Colloidal dispersions
- Surfactants, emulsions
- Pharmaceuticals
- Liquid crystals
- Porous materials
- Polymers, fibers

[1] Franke, D., Svergun, D.I., J. Appl. Cryst. 42 (2009) 342 ff. [2] Svergun, D.I. et al., J. Appl. Cryst. 45 (2012) 342 ff.
[3] Madl, T. et al., Molecular Cell 53 (2014) 941 ff.

Software

Dedicated software – ensuring the best SAXS/WAXS results

The SAXSpace system includes intuitive, user-friendly, and comprehensive software packages for system control, data acquisition as well as for fast processing and analysis of multiple SAXS and WAXS data.

SAXSdrive™: System control and data acquisition

SAXSdrive™ provides full control of all SAXSpace system components. It allows you to easily program and run automated SAXS/WAXS experiments.

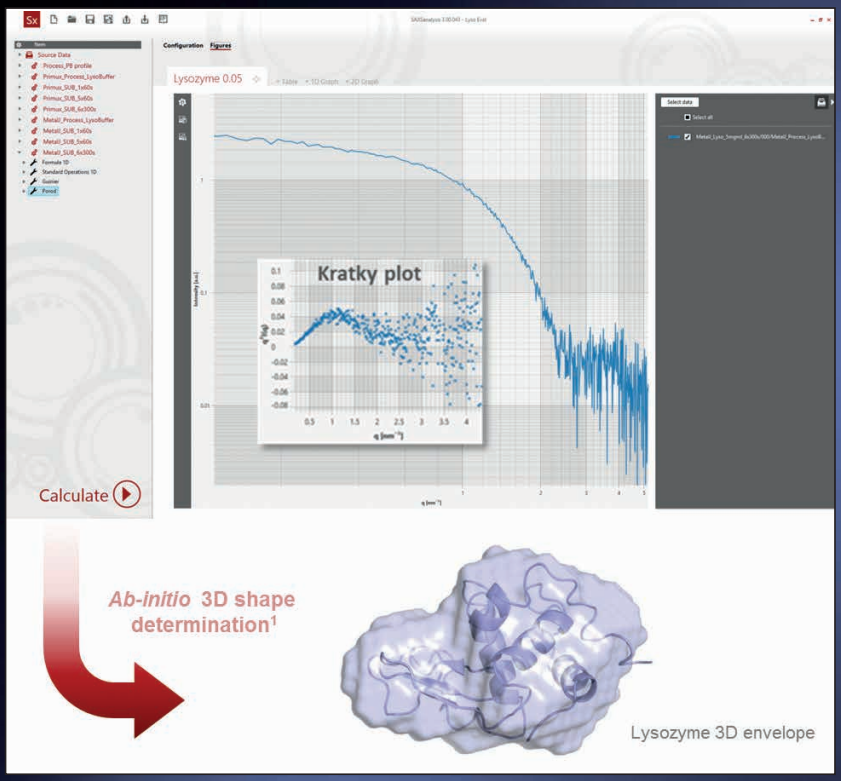
SAXSanalysis™: Data processing and analysis

SAXSanalysis™ is a comprehensive data reduction and analysis package for 2D and 1D scattering data. Fully customizable templates and a batch processing concept allow you to handle a large amount of data. The data layout follows the commonly used Nexus convention.

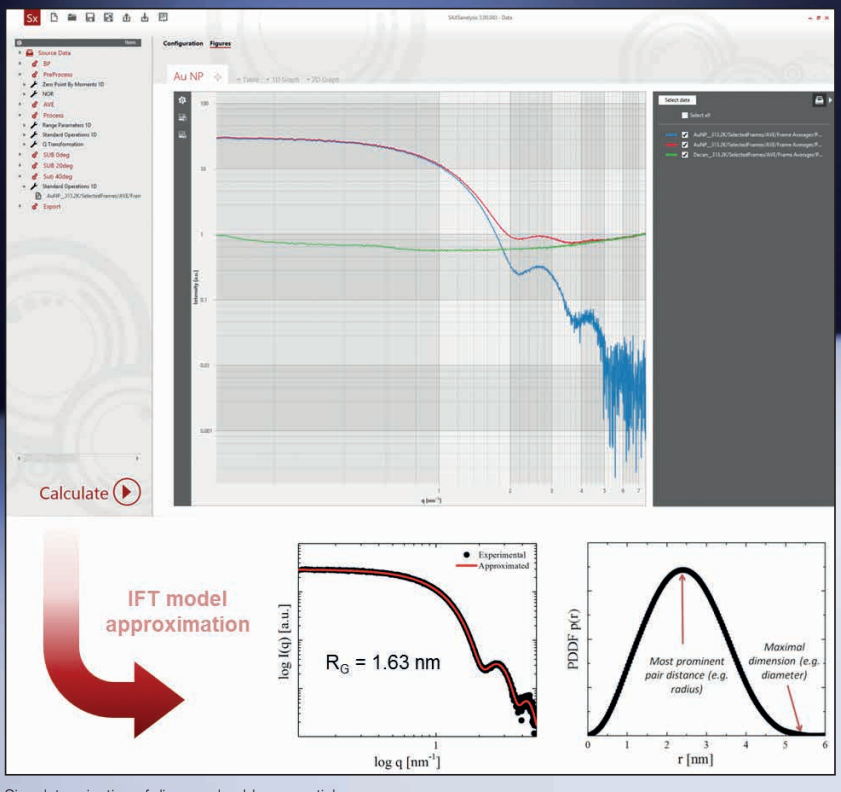
Determine important parameters and plots, such as radius of gyration RG, particle size, Porod constant, specific surface, and Kratky plots. Benefit from automatic data export routines to common IFT and model-fitting software packages (GIFT, ATSAS, SASfit, MacSAS, and others).

PCG: Advanced structure interpretation

Retrieve structural information such as particle size, size distribution, shape, and inner structure using IFT and deconvolution techniques. Interpret scattering data of interacting (i.e. concentrated or charged) particle systems.



BioSAXS: Determination of a 3D envelope



Size determination of dispersed gold nanoparticles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Automatic Experiment
Temperature
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Finally
Fit to Sci

Your SAXSpace system in good hands

Best quality

You can be sure that all components of your SAXSpace instrument are of the best possible quality. Anton Paar's long tradition, experience, and skills in producing high-precision measurement instrumentation for X-ray structure analysis ensure that your SAXSpace will produce high-quality SAXS/WAXS and BioSAXS results.

Profound SAXS/WAXS knowledge

We take care of your SAXSpace system: Starting with installation and commissioning of the system, our SAXS/WAXS specialists provide a thorough on-site user training to help you make the most of your SAXSpace system.

Application and service expertise

Anton Paar's worldwide network of experienced application and service specialists provides immediate support for the smooth operation of your SAXSpace instrument. Based on 60 years of SAXS experience we accompany you with dedicated technical and application support made available by our skilled SAXS/WAXS application scientists.

System specifications

X-ray source	Primux 3000 sealed-tube X-ray source (Cu, Mo)
X-ray optics and collimation	- Custom-designed multilayer optics (fully evacuated) - Automated scatterless Kratky-based block beam collimation (fully evacuated)
Sample stages and autosamplers	- TCStage temperature-controlled stages - Temperature-controlled autosamplers for multiple samples - ASX autosamplers for up to 192 liquid samples - Humidity Stage - GISAXS stage with heating/cooling option (-150 °C to 500 °C) - Tensile stage with heating/cooling option (-150 °C to 350 °C) - Customized solutions available on request
Special features	- TrueFocus: automatic self-alignment - TrueSWAXS: continuous and simultaneous SWAXS studies up to 60° 2θ - Stagemaster: YZ stage with auto-recognition of sample stages
Temperature range Atmosphere	- -150 °C to 600 °C - Temperature accuracy: ±0.1 °C - Vacuum, air, inert gas, humidity (reactive gases on request)
Sample holders	- Quartz capillary for liquids - Low-parasitics SiN Cell (point-collimation mode only) - Sample holders for solids - PasteCell for viscous and powder samples - RotorCell for sample spinning - High-pressure cells - µ-Cell for small sample volumes - FlowCell and TubeCell for automation - Osmotic cell - Heated sampler - Customized solutions available on request
Detectors	1D Mythen2 R series and 2D EIGER R series HPC detectors q_{min}: 0.03 nm^{-1} and q_{max}: 40.7 nm^{-1} (60° 2θ)
Software	- SAXSdrive™ measurement and acquisition software - SAXSanalysis™ data processing and analysis software - PCG advanced data interpretation software
Footprint	1.8 m x 0.9 m (L x W)

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