Introduction

SAXSpace is a lab-scale system for SAXS and WAXS studies. It determines the size, size distribution, and shape of nano-sized particles and intermolecular domains. Small-angle X-ray scattering studies of biological materials provide unique structural information and therefore complement other techniques, such as protein crystallography, NMR, and electron microscopy. With SAXS/WAXS, biological macromolecules and their complexes are investigated at 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.

Features of the Anton Paar SAXSpace

Large experimental temperature ranges

Sample chamber Peltier temperature controls ranging from - 30°C to 150°C and autosampler ranging from 4°C to 25°C for up to 192 liquid samples.

X-ray Source and Detectors

Primux 3000 sealed tube (Cu, Mo) source with 1D Mythen2 R series and 2D EIGER R series HPC detectors with either line or point collimation with resolution q_{min}: 0.03 nm^{-1}.

Accessible q range

0.03 nm^{-1} to 40.7 nm^{-1}

0.15 nm < d < 200 nm

Removable Sample Holders

- 1 mm quartz capillary (60 µL) for liquids
- µ-Cell (10 µL) for low volume liquids
- PasteCell for viscous and powder samples
- RotorCell for averaging microcrystalline domains
- TubeCell with flowthrough connetions (disposable fluid pathway)
- TCS Capillary Holder for disposable capillaries

Structural & Biophysical Core Facility

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Produced by Brandon Cordeiro

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Structural and Biophysical Core Facility

Automated Small / Wide Angle X-ray Scattering

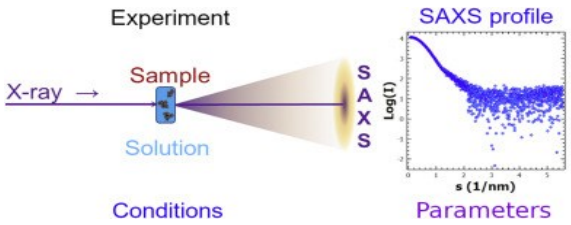
- Determine the size (r_H , r_G), shape, internal structure, porosity, orientation, and crystallinity
- Simultaneous SAXS (Bio-SAXS) and WAXS analysis
- Line collimation and point collimation
- Compatible with: colloidal dispersions (nanocrystals/pigments/metals), surfactants (detergents/food additives), emulsions (drug carriers/cosmetics), proteins, lipids, peptides, synthetic fibres, nano-composites (polymer/clays/carbon nano-tubes), and liquid crystals (detergents/food/biological membranes)

Anton Paar SAXSpace - Protein Shape Determination

Theoretical Background

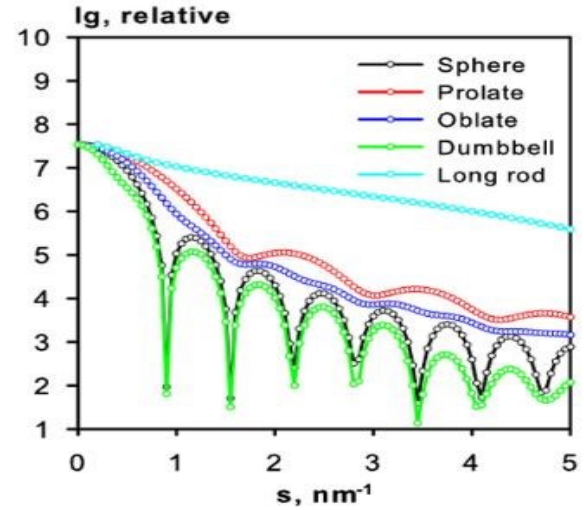
Small-angle X-ray scattering (SAXS) is a technique which quantifies nanoscale electron density differences in a sample material. SAXS measures the X-ray scattering intensities by a sample as a function of the scattering angle which ranges from as little as 0.1° to 10°.

From Bragg's law it is understood that with decreasing scattering angle, increasingly larger structural features are being probed. A SAXS signal is observed whenever a material contains structural features on the length scale of nanometers, typically in the range of 1-100 nm.



On the other hand, wide-angle X-ray scattering (WAXS), also known as wide-angle X-ray diffraction (WAXD), probes for structures in the material on the much smaller length scale, that of interatomic distances.

Based on the unique scattering profile (form factor) obtained, the morphology of the protein or protein assembly in solution can be revealed. With this information equipped with other analytical techniques, such as the ab-inition method, the 3D envelope of the sample can be modeled. This information is extremely useful in understanding biological function and examples of these form factors are displayed in the following figure.

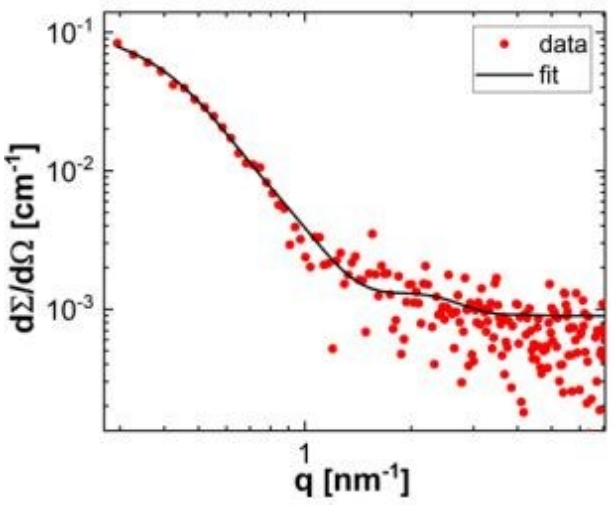


Organic Nanoparticle Analysis in Solution by SAXS

Sample: 1 mg/mL Co Enzyme Q10
Buffer: 208 µM SDS in Acetone
Exposure Time: 4 hours

Small angle X-ray scattering (SAXS) measurements were performed using the SAXSpace laboratory instrument. The sample was measured in a standard quartz capillary at 22 °C without further preparation. The sample-detector distance was 307 mm. The measurement signal of the dispersion medium was subtracted from that of the sample.

The SAXS curve was evaluated using a spherical shell model and a logarithmic particle size distribution. The SAXS data of the sample and a fit to the data based on a model of spherical core-shell particles is depicted in the following figure. The resulting radius of gyration was determined to be 19 nm. Both the radius of gyration and the hydrodynamic radius can be estimated using the available Anton Paar software package SAXSquant.



The radius of gyration is the distance from the center of mass of a body at which the whole mass could be concentrated, in a sense it's a mass average radius. The hydrodynamic radius, often called the stokes radius, relates to a perfect sphere moving through a solution resisted by the solution's viscosity. The speed at which the particle (Sphere) is moving is related empirically to the size at which a perfect sphere would move in the same experimental conditions.

Both radii can be extracted from the data points (red) displayed in the above figure after a few processing steps available in the SAXSquant software. The 3D envelope can then be estimated using both of these values along with external software (DAMMIF) and is shown in the example figure to the right of this text.