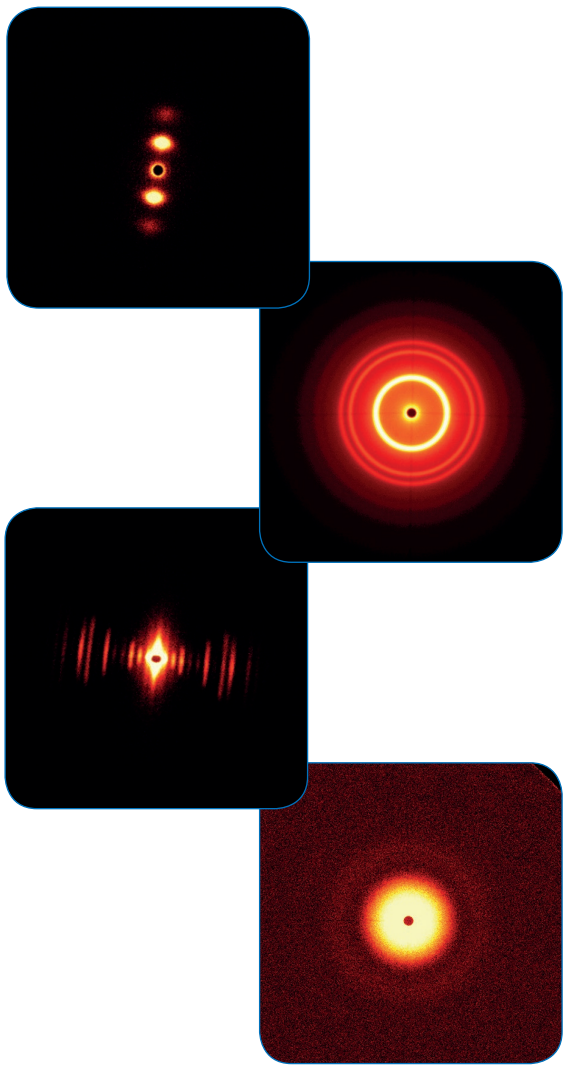
DIFFRAC.SAXS

Comprehensive SAXS Analysis

DIFFRAC.SAXS sets a new benchmark for Small Angle X-ray Scattering (SAXS) software. Interpretation of 1D and 2D SAXS data has never been easier, faster and more accurate.
DIFFRAC.SAXS combines an extensive collection of modern and powerful algorithms for data processing and evaluation with a work-flow that is simple and flexible. Seamless integration of each step in the visualization, data reduction and analysis process ensures ease of use and accurate results. Many operations can run automatically to maximize throughput, or interactively for ultimate control.
DIFFRAC.SAXS has different data analysis routines onboard, including model-free as well as model-based methods, to cope with the huge diversity of nanomaterials.
DIFFRAC.SAXS features an easy-to-use user-interface, advanced graphics and customizable analysis report.
An extensive step-by-step tutorial considerably shortens the learning curve. The tutorial and extended user manual also serve as excellent tools to introduce newcomers to SAXS analysis, getting them started in the shortest time possible.



- Seamless integration of data visualization, pre-processing and evaluation
- Advanced data evaluation through model-free and model-based routines
- Automated as well as interactive operation

DIFFRAC.SAXS is a comprehensive software suite for analyzing SAXS data. This includes data visualization, data pre-processing, and subsequent data evaluation.

Import and visualization

DIFFRAC.SAXS displays 1D and 2D SAXS data, as well as Nanography maps. Supported data formats are brml, raw, ascii (two-column xy and three-column xye with different units), gfrm and tiff.

Data pre-processing

Proper pre-processing of the measured data is essential for successful SAXS analysis. DIFFRAC.SAXS allows extracting the pure scattering signal of the nanostructures straightaway.
In a first step the sample transmission is determined using glassy carbon as reference, or based on the primary beam intensity ratio. 2D data are subsequently sliced or integrated through optimized algorithms into 1D data for further evaluation. In particular for weakly scattering samples accurate background correction is a must.
DIFFRAC.SAXS can perform both the transmission calculation and the background correction automatically, without the need for user intervention, if the data measurement strategy is set up with DIFFRAC.WIZARD.

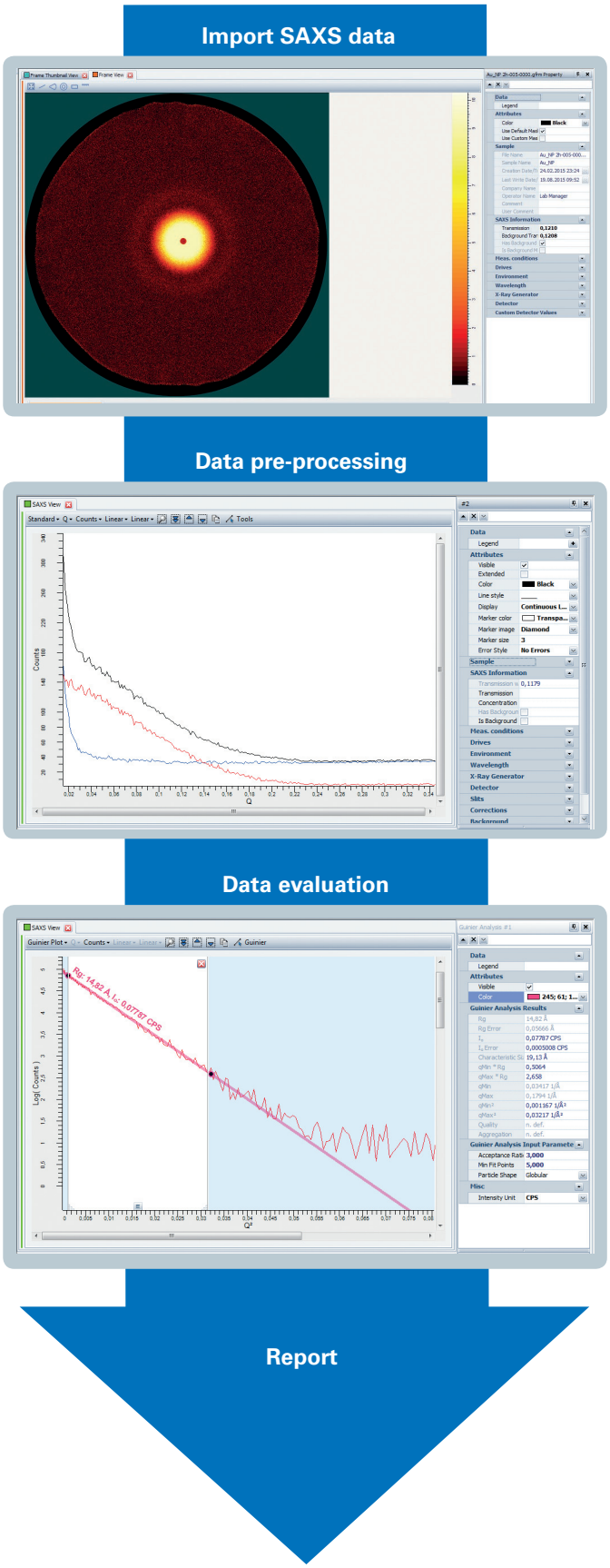
SAXS specific plots and evaluations

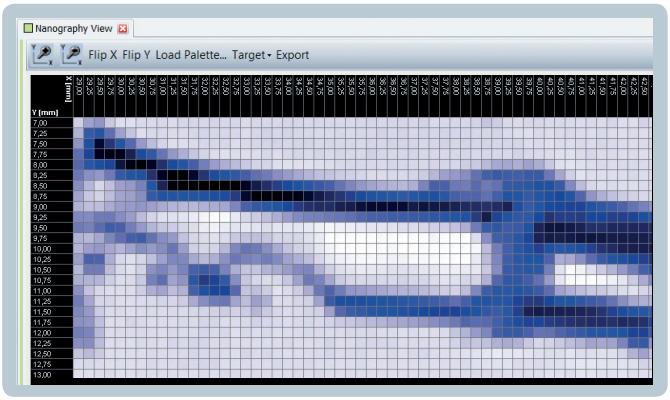
Traditionally, SAXS curves are displayed as plots with specific axis scaling that allow a quick graphical check of the data quality, and straightforward parameter evaluation. These specific SAXS plots are essentially the Guinier, Porod and Kratky plots. In DIFFRAC.SAXS all plot types can be readily selected by name. Evaluation of the related parameters, such the radius of gyration, the forward scattered intensity, the Porod scattering invariant, surface-to-volume ratio etc. is done fully automatically or interactively in a step-by-step procedure.

Scaling to absolute units and molecular weight calculation

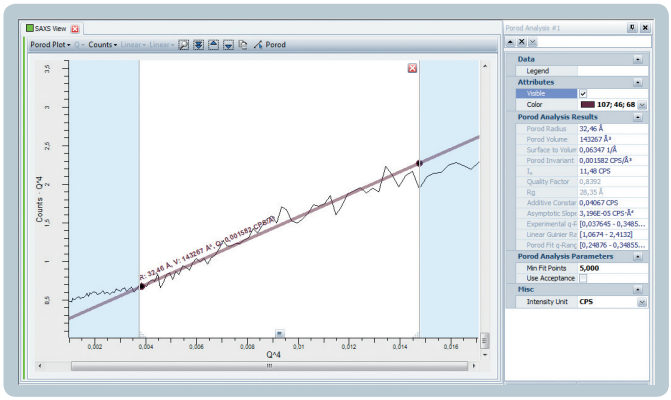
The measured SAXS data can be further scaled to absolute units in DIFFRAC.SAXS based on SAXS data from a standard with known scattering cross section, such as water. Scaling to absolute units is a prerequisite for advanced data analysis, e.g. for determining the molecular weight of proteins. Alternatively the molecular weight can also be determined based on SAXS data from a reference protein with known molecular weight.

SAXS analysis workflow





Nanography map



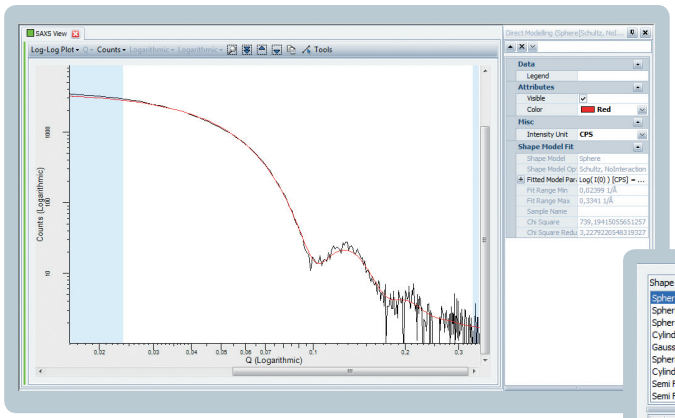
Porod analysis

Model-based fitting

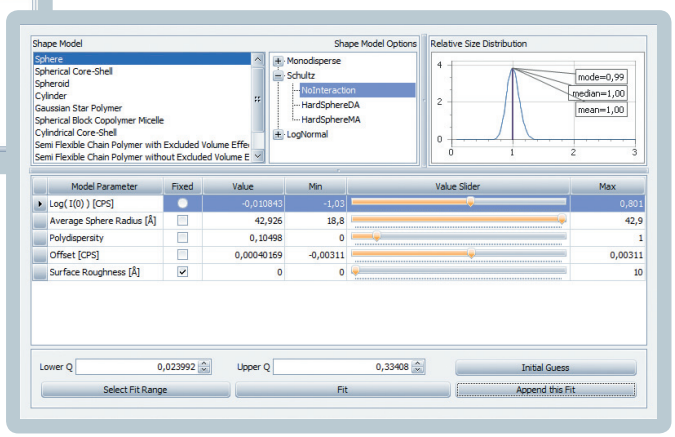
DIFFRAC.SAXS features a non-linear least-squares fitting of 1D SAXS data based on direct modeling of nanostructures in solution using geometrical shapes (sphere, cylinder, etc.) or by dedicated polymer models (chains, Gaussian star, etc.). It also takes into account polydispersity and concentration effects for complete sample characterization. The corresponding model parameters are determined by fitting the experimental SAXS curve.

Pair Distance Distribution Function

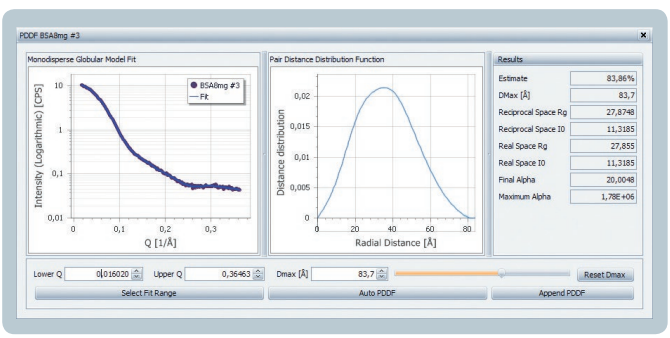
The Pair Distance Distribution Function (PDDF) p(r) is the distribution of the distance taken between any two points within the scattering particle. The PDDF is function of the size and shape of the particle, and relates to the scattering curve by a sin Fourier transform. DIFFRAC.SAXS allows retrieving the PDDF from the scattering curve based on GNOM routines from the well-known ATSAS* suite.



Model fit of gold nanoparticles with a spherical model, Schulz distribution without particle interaction



Model fit tool box



PDDF analysis of BSA protein

* ATSAS is a program suite for SAXS data analysis copyright protected by EMBL, and licensed by Bruker.

Data import

- Import of 1D data files (. raw, .xy, .xye, .dat, .txt or .ssd format)
- Import of 2D data files (.brml, .gfrm or .tiff format)
- Nanography maps as .brml files

2D Frame data processing

- Masking, slicing, averaging
- 2D frame integration over gamma and 2Theta with full frame, wedge, ring and line cursor
- Frames are automatically grouped into mergeable or stackable lists
- Multiple integrations on stackable 2D frames with one click
- For large zoom factors the 2D view displays the number of counts inside the pixel areas

1D Scan display

- Pre-selected settings for scan display: Log-Log, Guinier- , Porod and Kratky Plot
- Options for the standard view: the x-axis can be changed by selecting 2θ, q, q^2, q^4, 1/d or d.
- The scaling of the x-axis can be set to linear, square root, logarithmic, square or inverse
- The scaling of the y-axis can be set to linear, square root or logarithmic
- Customization of graphics and text properties for creation of publication-ready figures

1D Data processing

- Addition, subtraction, cumulating, scaling, normalization and merging of scans
- Data resampling
- Shifting the momentum transfer
- Scaling and shifting the intensity
- Sample transmission evaluation
- Interactive and automatic background subtraction
- Extrapolation to zero concentration
- Putting intensities on absolute scale
- Computation of statistical errors

SAXS Global Structural Parameters

- Interactive and automatic Guinier analysis providing radius of gyration, forward scattered intensity, etc.
- Interactive or automatic Porod analysis providing the Porod scattering invariant, surface-to-volume ratio, etc.
- Kratky analysis
- Molecular weight of proteins
- Pair Distance Distribution Function (PDDF)

Model-based fitting

- Non-linear least-squares fitting of 1D SAXS data based on nanoparticle shape models, taking into account polydispersity and interaction effects
- Available shape models: sphere, spherical core-shell, spheroid, cylinder, and cylindrical core-shell
- Available polymer models: Gaussian Star polymer, semi-flexible chain polymer with and without excluded volume effects, flexible chain polymer with and without excluded volume effect
- Gaussian, Lognormal and Schultz-Zimm distribution

Data exchange and reporting options

- Creation of customizable, high quality analysis reports
- Data exchange options to and from any other Windows application: copy and paste, Windows bitmaps and metafiles
- Export of measured and pre-processed data as Bruker's .raw file format, and ASCII (2 column XY or 3 column XYE format)
- Export of results for further evaluation in other SAXS software, e.g. GNOM.out file for further evaluation with ATSAS

Operating system

- Windows 7 or 8 (32 Bit or 64 bit)

Bruker AXS GmbH

Karlsruhe · Germany
Phone +49 721 50997-0
Fax +49 721 50997-5654
info.baxs@bruker.com

www.bruker.com