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EASYSAXS SOFTWARE

Analysis of small-angle X-ray scattering (SAXS) data

Determination of nanoscale structures and dimensions

EASYSAXS - SIMPLY POWERFUL

Advanced software for the analysis of small-angle X-ray scattering (SAXS) data

EasySAXS - suitable for experts and beginners alike

EasySAXS is an advanced, user-friendly software package for the analysis of small-angle X-ray scattering (SAXS) data. It allows to deduce information on nanoscale structures and dimensions, nanoparticle shapes and surface areas.

EasySAXS offers a complete data analysis toolbox, automation options and reporting. The toolbox includes data reduction, Guinier and Porod analyses, pair distance distribution function determination, least-squares fitting and model simulations. All parameter settings are conveniently accessible in the graphical user interface allowing for efficient data analysis. Data can be exported in a format that is compatible with publicly available SAXS software packages that give access to extended analysis.

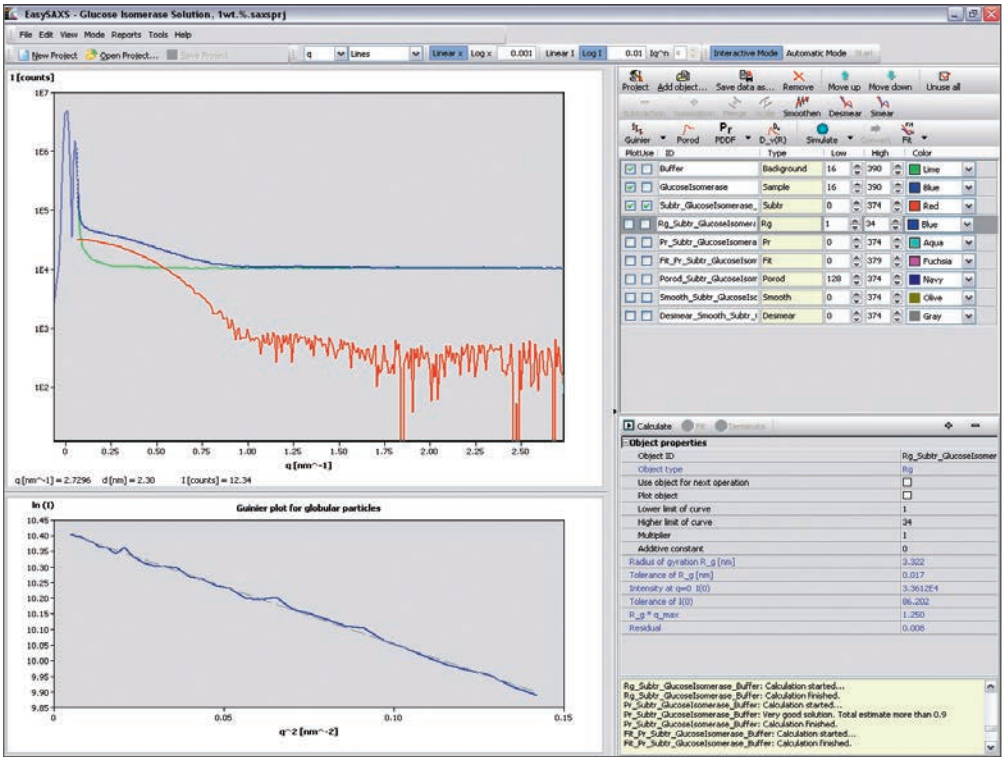
A collaboration with world-class scientists at the EMBL

Some of the algorithms used in EasySAXS are based on codes from the renowned ATSAS software suite developed by Dr. Dmitri Svergun and his team at the European Molecular Biology Laboratory (EMBL) in Hamburg, Germany. These include pair distance distribution function and particle size distribution analyses enabled by indirect Fourier transformation calculations.

EMBL

User interface

The graphical user interface of EasySAXS facilitates particularly easy and efficient access to all software functionalities and parameter settings.



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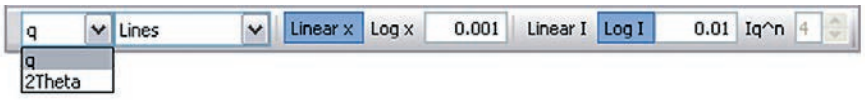
Data display

Experimental SAXS data and analysis results are shown in two zoomable graphics panes. The position of the mouse on the graph is indicated with a crosshair and the corresponding numerical values (q or 2θ, Bragg spacing d and intensity) are given below the graph.



Choose your preferred abscissa
- Scattering vector q (in units of Å^{-1} or nm^{-1})
- Scattering angle 2θ

$$q = \frac{4\pi}{\lambda} sin\left(\frac{2\theta}{2}\right)$$
Scattering vector

$$d = \frac{2\pi}{q}$$
Bragg spacing

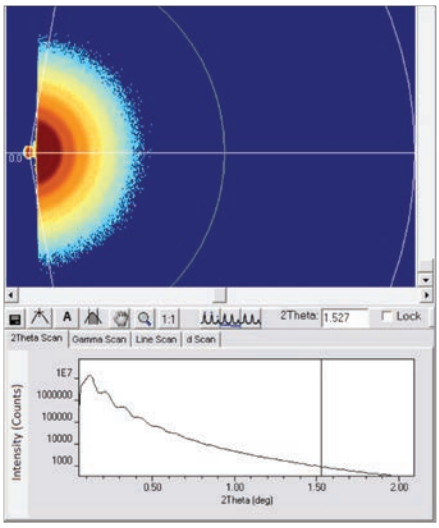
Data display options include
- lin / log - the default option
- log / log - reveals characteristic scaling behavior in the data
- Guinier plot - (ln$I$ vs. q^2) to analyze the curvature of the scattering curve at smallest angles
- Porod plot - (Iq^4 vs. q, or Iq^3 vs. q) to analyze the final slope of the scattering curve
- Kratky plot - (Iq^2 vs. q) used for BioSAXS data to investigate for protein folding / unfolding

Import of data files – maximum flexibility

EasySAXS can import SAXS data that were acquired with Data Collector using any of PANalytical's SAXS setups, and supports all types of suitable measurement programs.

The software also reads in columnar ASCII files containing SAXS data that were acquired using other lab instruments or a beamline at a synchrotron radiation facility.

XRDML - PANalytical's open XML file format



2D SAXS data can be pre-processed in PANalytical's XRD2DScan software and then exported for further analysis with EasySAXS.

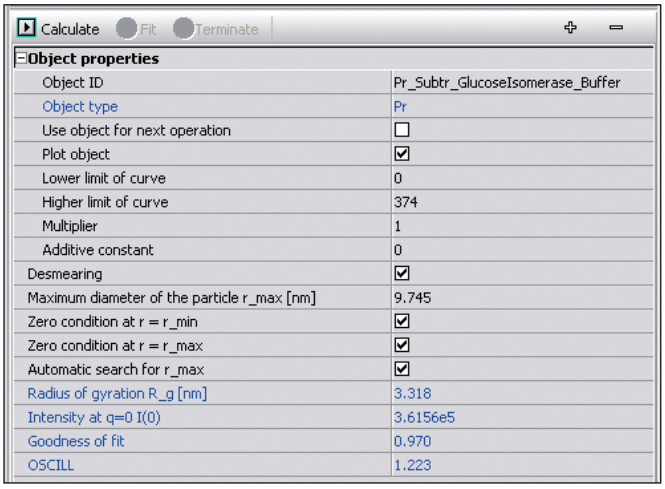
Data reduction and treatment options

EasySAXS enables you to perform a variety of initial data reduction and data treatment operations:

- **Background subtraction**, by properly taking into account the attenuation by the sample
- **Summation** of individual scans, e.g. from a set of repeated measurements
- **Merging** of experimental data, that were e.g. acquired from a given sample at lower and higher concentrations
- **Scaling** of scattering curves to the same intensities within a user-defined angular range
- Data **smoothing** in intervals, if desired
- **Desmearing** (or **smearing**) of data, to take into account effects due to the finite dimensions of the X-ray beam

Define parameters and inspect analysis results

In the Object Inspection pane you can conveniently set the parameters for a calculation. In many cases the default settings are already suitable. The results from data analysis are also displayed in this pane.



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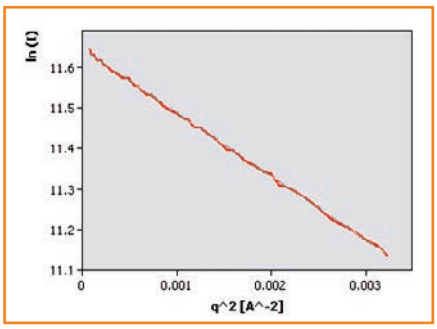
Data analysis options

EasySAXS offers a comprehensive toolbox for the analysis of SAXS data. The options range from the model-independent determination of size and structure parameters, to fitting and simulation based on models assuming a specific particle shape.

Guinier analysis

Use a Guinier plot for the analysis of the initial curvature of the scattering curve, to determine the **radius of gyration R_g**. **Extrapolate** the data to 0° 2θ for obtaining the forward scattering intensity ***I(0)***. Investigate for nanoparticle **agglomeration** effects. For strongly anisometric particles, determine the radius of gyration of the cross section (in case of cylinders) or of the thickness (in case of platelets).



Guinier plot for globular particles

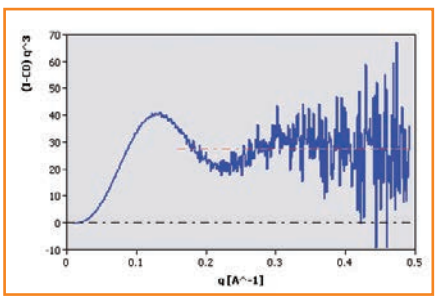
$$I(q) = I(0)\exp(-q^2 R_g^2 / 3)$$

Guinier's Law

Object properties	
Object ID	Rg_ColloidalNanospheres
Object type	Rg
Use object for next operation	☐
Plot object	☐
Lower limit of curve	3
Higher limit of curve	55
Multiplier	1
Additive constant	0
Radius of gyration R_g [A]	21.755
Tolerance of R_g [A]	0.038
Intensity at q=0 I(0)	1.1425E5
Tolerance of I(0)	90.535
R_g * q_max	1.232
Residual	0.004

Porod analysis

Use a Porod plot to analyze the final slope of the scattering curve and to **extrapolate** the data towards high scattering angles. Determine the **Porod constant** and calculate the **scattering invariant** *Q*, to estimate **specific surface areas** and the **Porod volume** of nanoparticles.



Porod plot

$$Q = \int_0^{\infty} I(q) \cdot q^2 \, dq$$

Scattering invariant

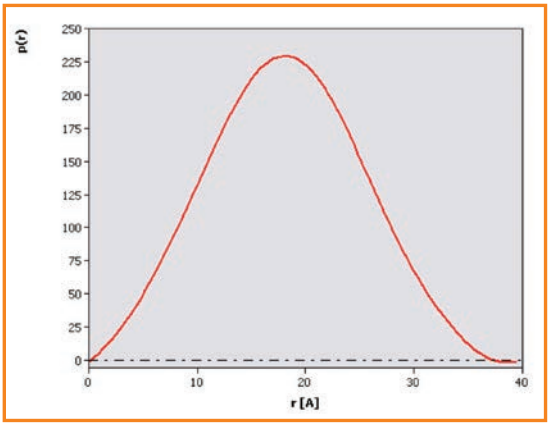
Object properties	
Object ID	ColloidalQuantumDots
Object type	Porod
Use object for next operation	☐
Plot object	☐
Lower limit of curve	160
Higher limit of curve	517
Multiplier	1
Additive constant	0
Input data property	Smeared
Calculate invariant Q using linear extrapolation	☑
Porod constant k	27.750
Estimate C0	☑
Background constant C0	-9.925
Error estimation for Porod approximation	9.256
Invariant Q	593.451
Surface-to-volume ratio S/V [A^-1]	0.1070
Porod volume V_p [A^3]	0

Data analysis options

Pair distance distribution function *p(r)*

The *p(r)* function is the real space counterpart of the intensity curve *I(q)*. EasySAXS calculates *p(r)* by an **indirect Fourier transformation** of the intensity data. Artifacts due to statistical noise and due to termination effects are thus minimized, and the most stable solution is automatically selected based on perceptual criteria. Smearing effects can directly be taken into account in these calculations.

Use *p(r)* analysis in case of well-defined, monodisperse particles (e.g. proteins) to determine the **maximum particle dimension D_{max}** and to deduce information about the **particle shape**. Furthermore, **the radius of gyration R_g** as well as the forward scattering intensity ***I(0)*** can be determined from the *p(r)* function.



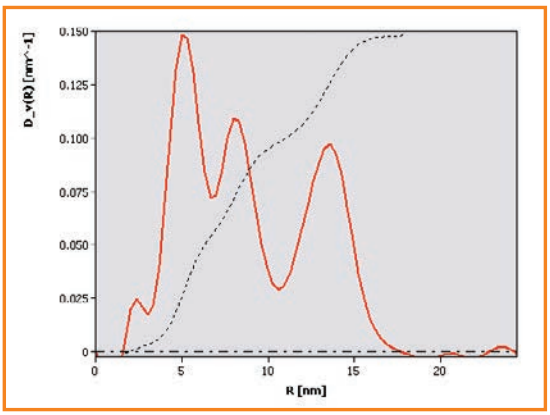
Pair distance distribution function p(r) calculated for a protein sample based on a measurement that was performed with ScatterX78 (lysozyme solution, 1 wt.%). It can be concluded that the protein has a globular shape and a maximum dimension of 38 Å. The p(r) function can be used for more in-depth analysis, such as ab initio protein shape reconstruction.

$$I(q) = 4\pi \int_0^\infty p(r) \frac{\sin(qr)}{qr} dr$$

Pair distance distribution fct. *p(r)*

Nanoparticle size distribution analysis

Using the indirect Fourier transformation algorithm, it is also possible to analyze the size distribution of spherical nanoparticles. Compared to model fitting this approach has the advantage that no *a priori* assumption about the shape of the size distribution curve has to be made. In this way also multi-modal particle size distributions can be revealed.



A trimodal nanoparticle size distribution as determined by indirect Fourier transformation

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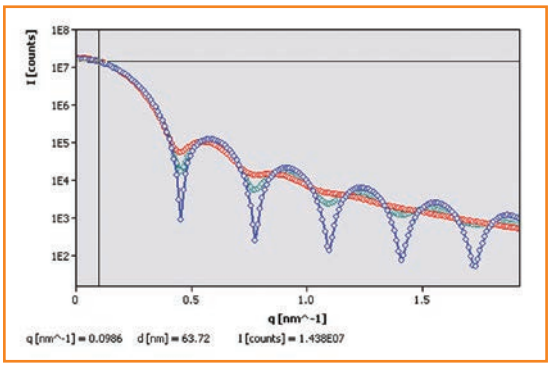
Simulation and model fitting

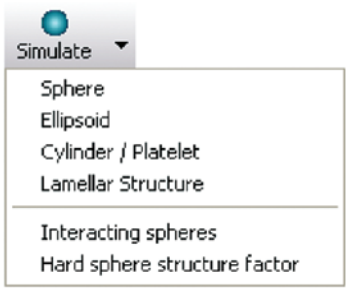
EasySAXS supports model simulations and fitting for a variety of nanoparticle shapes and structures. These calculations can take into account size polydispersity effects as well as core-shell structures with multiple shells. The instrumental smearing effects can directly be included in these calculations, thus making prior desmearing of the data to be fitted unnecessary.

$$I_{sp}(q) = I(0) \cdot \left[3 \frac{\sin(qR) - qR\cos(qR)}{(qR)^3} \right]^2$$

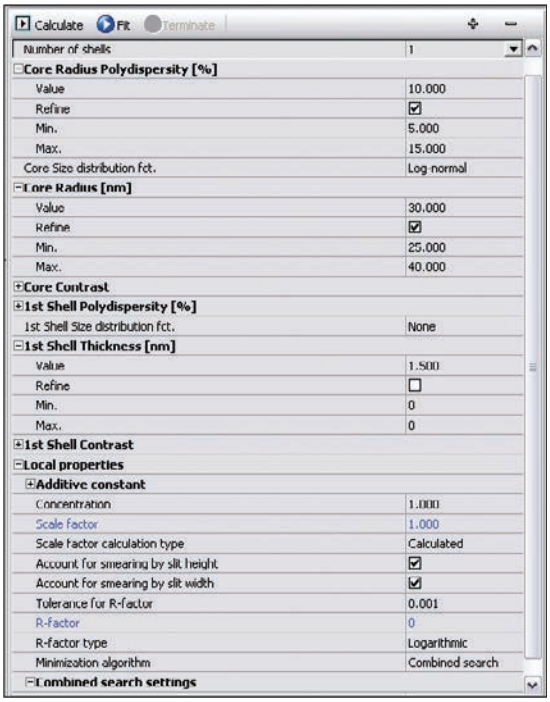
Scattering from a sphere

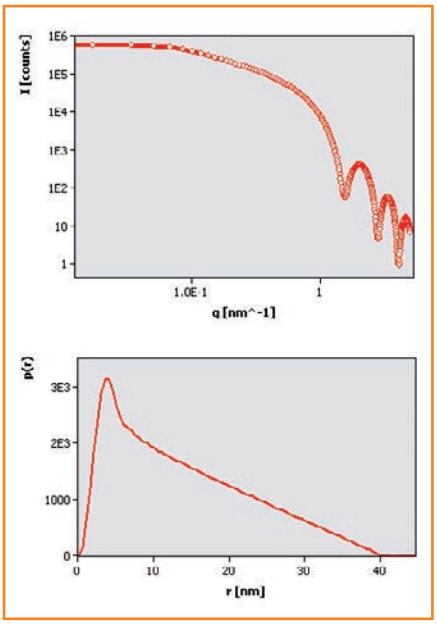


Simulation of SAXS data for ensembles of spherical particles with different size polydispersity



The user interface allows to easily define the individual model parameters, to select the parameters to be fitted, as well as to define fitting constraints. Furthermore, users have the option to choose between different minimization algorithms and R-factor types.

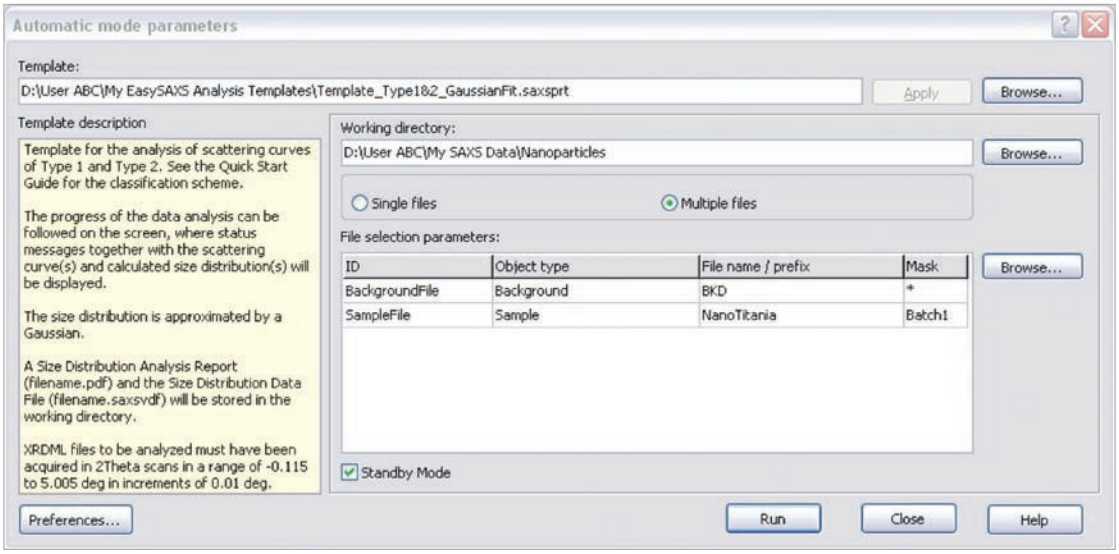




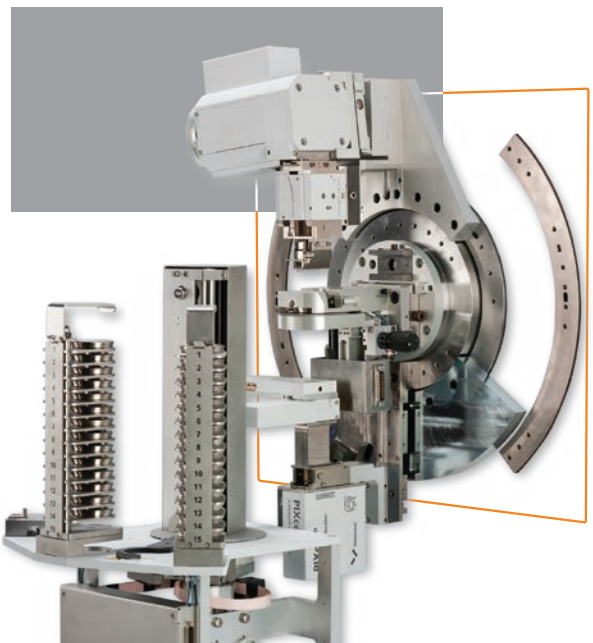
Example of a simulation of SAXS data from cylindrical nanoparticles and calculation of the corresponding pair distance distribution function p(r)

Automation options

Beginners and less experienced users can get started quickly by using the automatic mode of EasySAXS. It enables automated particle and pore size distribution analysis of multiple data files by applying analysis templates that contain pre-defined parameter settings.
A variety of analysis templates, applicable for different sample types, are delivered with EasySAXS. Users can also create their own templates for specific samples of interest.



Setup window in the automatic mode



SAXS setup with an automatic sample changer allowing for measuring a complete batch of samples

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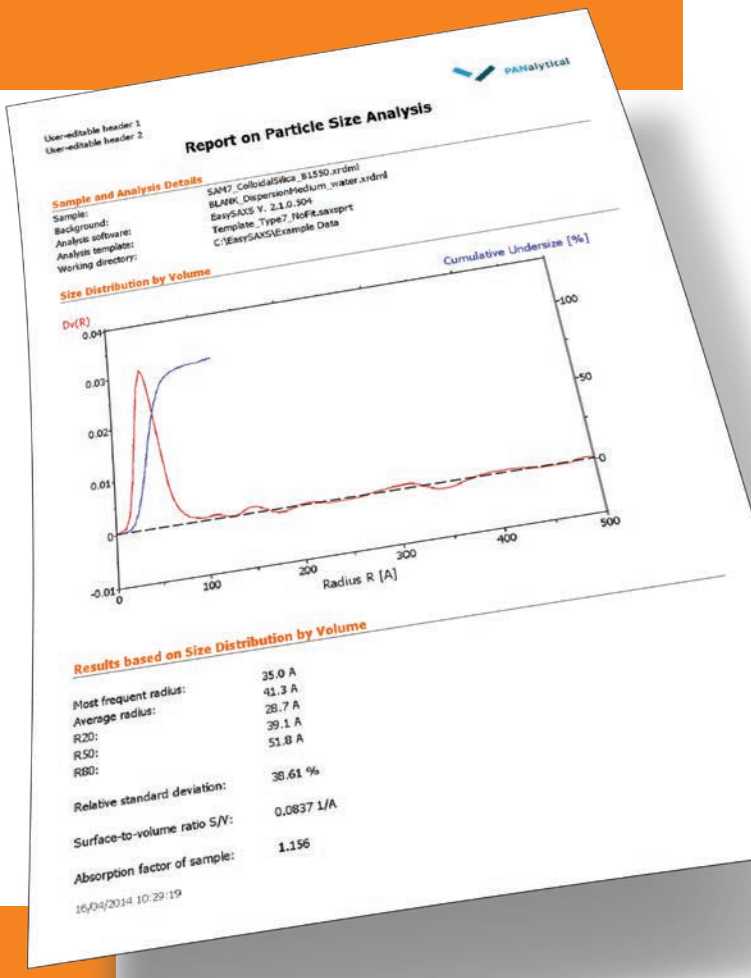
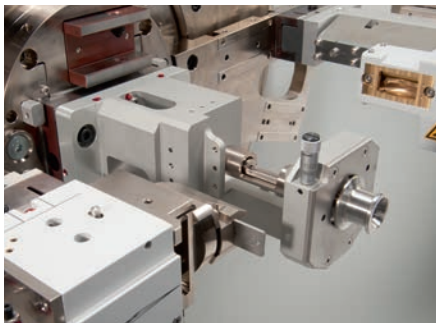
Reporting

For the size distribution analysis of nanoparticles it is possible to create customizable reports. When using the automatic mode of EasySAXS, these are created automatically.





Multipurpose SAXS/WAXS stage

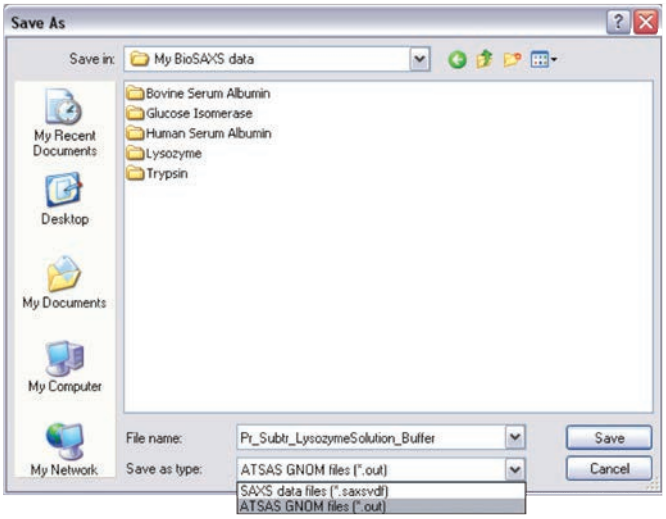
Message pane

Follow the progress of calculations and get hints and warnings, when necessary.

```
Pr_Subtr_GlucoseIsomerase_Buffer: Calculation started...
Pr_Subtr_GlucoseIsomerase_Buffer: Very good solution. Total estimate more than 0.9
Pr_Subtr_GlucoseIsomerase_Buffer: Calculation finished.
Fit_Pr_Subtr_GlucoseIsomerase_Buffer: Calculation started...
Fit_Pr_Subtr_GlucoseIsomerase_Buffer: Calculation finished.
Rg_Subtr_GlucoseIsomerase_Buffer: Calculation started...
Rg_Subtr_GlucoseIsomerase_Buffer: q_max * Rg > 1.3. The higher limit must be reduced.
Rg_Subtr_GlucoseIsomerase_Buffer: Calculation finished.
```

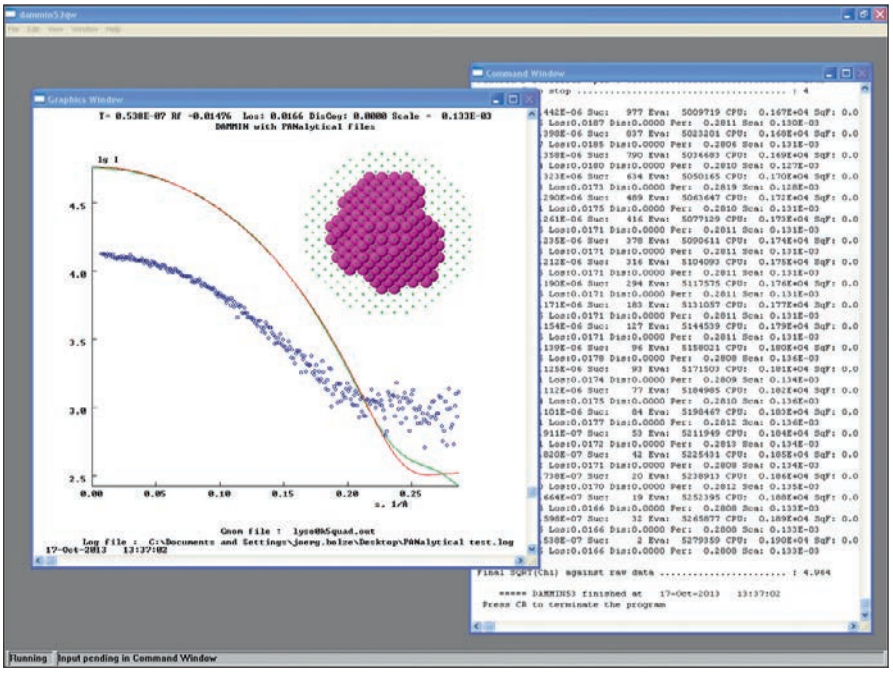
Data export

If desired, all data can be exported for further processing or display with other publicly available software (such as ATSAS, Irena, SASfit).



Compatible with the ATSAS package from EMBL

ATSAS is a popular program suite for small-angle scattering data analysis from biological macromolecules. The software was developed by Dr. D. Svergun and his team at the European Molecular Biology Laboratory in Hamburg, Germany. Experimental SAXS data acquired with ScatterX[78] from dilute protein solutions can be pre-processed with EasySAXS and then exported to ATSAS for further in-depth analysis, e.g. *ab initio* **protein shape reconstruction**.



Shape reconstruction of a protein using DAMMIN from the EMBL ATSAS suite

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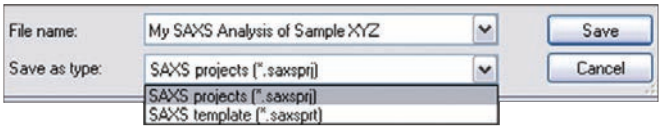
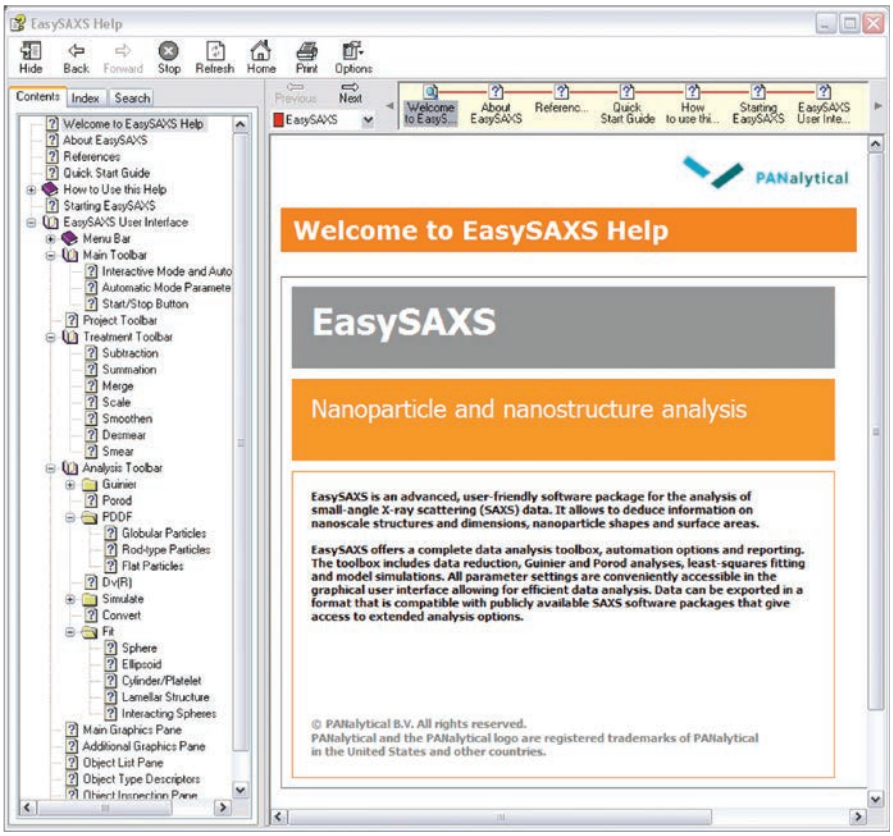
Save your analysis

All data analysis steps, including all details, can be stored in a **project file**. This allows to resume your analysis at a later point in time or to share your analysis scheme with others. The analysis strategy may also be saved in a **template file** that can later be applied to run a batch program in the automatic mode.



User documentation

EasySAXS contains a comprehensive, context-sensitive **Help system**. It includes step-by-step instructions for all tasks, parameter descriptions, theoretical background information, references to the scientific literature, as well as some worked examples. An additional **Quick Start Guide** helps you to explore the concept of using the software in the automatic and interactive modes.

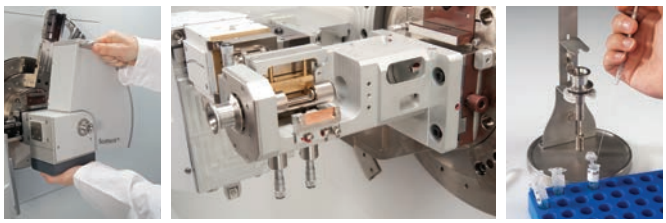


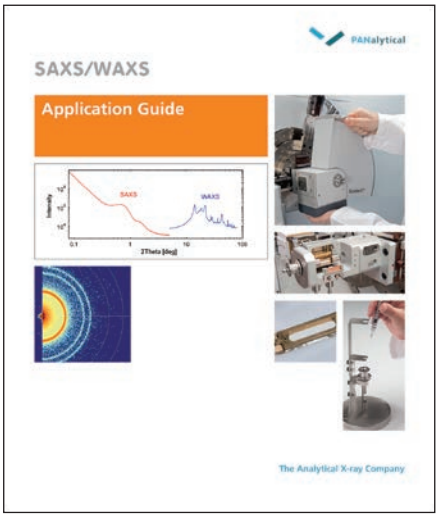
PANalytical provides complete SAXS/WAXS solutions

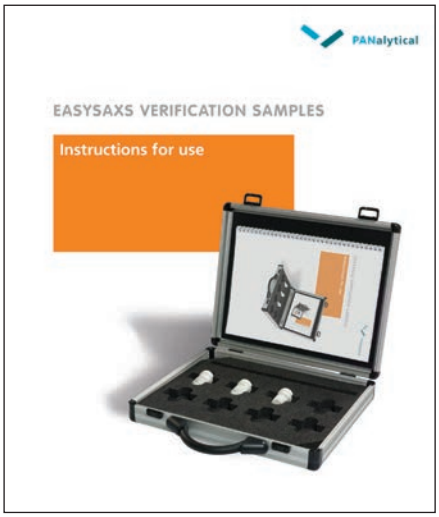
PANalytical has many years of experience in developing a range of highly cost-effective SAXS/WAXS solutions. These are typically being used at universities, in service labs and R&D departments, as well as for quality control.

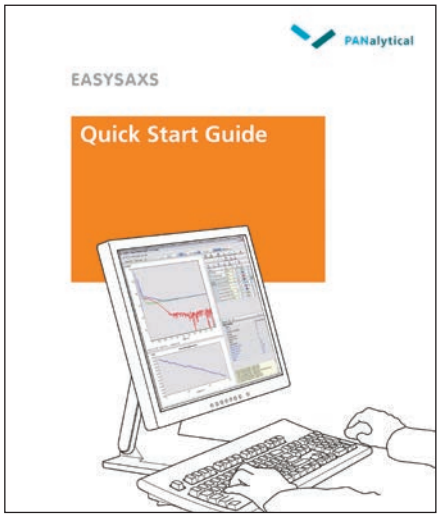
SAXS/WAXS measurements can be performed on our various multipurpose XRD platforms for which dedicated, pre-aligned hardware modules are available. Highest data quality, even for very weakly scattering and dilute samples, can be achieved with the **ScatterX^{78}** attachment that includes an evacuated beam path.

A dedicated **SAXS/WAXS stage**, designed for setups without a vacuum path, offers a more economical alternative. Both solutions also allow for 2D SAXS measurements. Entry-level SAXS/WAXS measurements are possible using sample stages and optics that are typically used for powder diffraction, and by just adding a few slits. Holders and sample preparation tools for powders, liquids and solid objects are available.





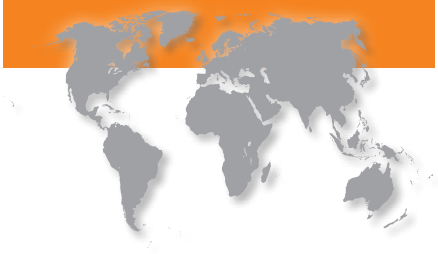




A SAXS/WAXS application guide helps you to get started quickly with measurements of your nanomaterial samples. A set of nanopowder samples is available for doing exercises and for verification purposes. The EasySAXS data analysis software, that comes with a Quick Start Guide and a concise Help function, makes the package complete.

All our solutions were designed with maximum ease of use in mind. Training courses are offered in our application laboratories worldwide, but can also be given at our customers on-site.

Global and near



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