Newsletter
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Editorial

Dear valued customers and partners,

The use of X-ray microsources is gaining pace day by day. Their vast field of application includes amongst others, single crystal, powder diffraction as well as Small Angle X-ray Scattering for nanomaterials studies.

Over the years, Xenocs has gained a reputation for the unmatched performances and reliability of its products among the SAXS and X-ray diffraction communities. In this issue we are pleased to share with you customer testimonials of our latest installations in these fields.

Xenocs is renowned for the quality of its customer support worldwide. In order to better serve our customers, we are constantly appointing new local distributors and provide them with continuous training on our latest products in order to better respond to your needs. In this news letter an update is given on our current distribution network and latest training session.

With this newsletter we share the experiences of our community of customers working with our products and the latest evolutions of our product lines. This newsletter is yours, so do not hesitate to share with us your suggestions for future editions.

Enjoy reading!

Frédéric Bossan
Executive Vice President - Marketing & Sales Director

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High performance SAXS/WAXS instrument with GeniX low divergence

Courtesy of Dr Roy Beck-Barkai from Tel Aviv University

A GeniX (50W, 50 µm) equipped with a FOX 3D 12_INF optic was installed in fall 2010 in Tel-Aviv University in the experimental biophysics laboratory of Dr Roy Beck-Barkai at the School of Physics and Astronomy, faculty of exact sciences on a small and wide angle x-ray scattering (SAXS / WAXS) laboratory beamline.

Dr Roy Beck-Barkai principal research interests are in the field of nanostrutured self assembled polymers and biopolymers, biophysics of supramolecular complexes, statistical mechanics and hydrodynamics of polymers, protein-protein and lipid-protein interactions. Among other techniques, SAXS and WAXS is the cornerstone of characterization of such systems, providing a direct insight of molecular organization and interactions, from the atomic level up to 100 nanometers or more. Using a SAXS/WAXS setup allow Dr. Beck-Barkai's team to directly probe the macromolecular forces and interactions with extended characteristics length-scales at hydrated condition.

In this SAXS/WAXS beamline (Figure 1), the GeniX low divergence system is coupled to two sets of scatterless slits collimation and two detectors are used to cover a wide range of measuring methods: a large Image Plate detector – MAR345 (Mar Research) is used for WAXS measurements and a high performance Pilatus 300K detector (Dectris) for SAXS measurements.

The quality of the GeniX low divergence arises from the combination of high brilliance microfocus source and single reflection aspheric multilayer optics to provide a highly parallel beam with high photon density. Despite using low power, its performance in SAXS is several times higher than standard sealed tube systems or traditional high power rotating anode generators due to very low divergence of the resulting beam.

The GeniX is coupled to a collimator made of two scatterless slits and a telescopic tube adapted to change the beam properties in a rapid and stable manner. The use of scatterless slits technology for beam collimation is a unique advantage in terms of brilliance preservation as a simplified collimation with only two slits is possible for high resolution SAXS [i]. The low scattering signal from the slits is also a benefit in terms of ease of alignment as no clean up adjustment is needed after

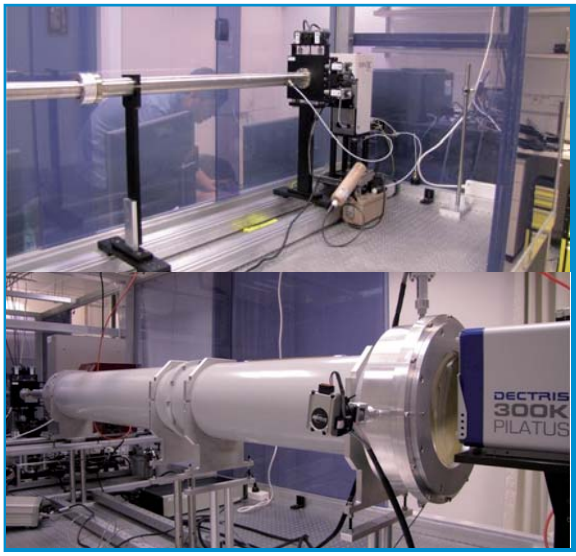


Fig. 1: View of SAXS beamline, seen from detector side.

Top: from left to right, GeniX beam delivery system, including the FOX3D 12-INF optic, the scatterless slit #1 and the vacuum tube.

Bottom: from left to right: the slit #2, the sample area, the WAXS detector MAR 345 Image Plate, the evacuated beam path, the motorized beam stop chamber in vacuum and reinforced exit window, the Pilatus 300K detector on a X-Z motorized platform.

changing beam size. The highly parallel and stable beam provided by the GeniX is also a key feature when reconfiguring the collimator length and slits aperture for different flux/resolution settings.

Depending on collimator length and slit size, typical flux range is 2.5x10^{7}-5x10^{7} photons/sec with 0.8mmx0.8mm beam size. The high quality of microfocus source is well demonstrated with the q_min = 0.044nm^{-1} (0.0044Å^{-1}) obtained with a long sample-to-detector distance of 2452mm as observed on Figure 2.

The SAXS/WAXS system is quite modular and with shorter diffracted beampath intermediate resolution (sample to detector distance of 1m) using the high sensitivity Pilatus detector can be achieved with a high flux. Such configuration is illustrated in Figure 3 with a 30 minutes measurement in a low scattering contrast sample (a lipid multi-lamellar vesicle sample).

To simplify WAXS studies and avoiding displacing the SAXS detector, a second large area plate detector (MAR345) is positioned close to the sample (27cm). This is greatly facilitated with the true parallel beam from GeniX low divergence and scatterless collimator, with low parasitic level: overlap with SAXS data is straightforward. Beam being stable in space, swap of detector is made in a snap, dedicated WAXS beamstop being already aligned from previous WAXS session and with only extremely limited mechanical maneuvers. For instance, with a large detector as such as the Mar345, sligthly offset and positioned at approximately 27cm offers q_range [0.04, 3.00]Å^{-1} or 2-theta [0.5, 43.0]°, as seen on Figure 4 for WAXS data on Ag Behenate sample.

Moreover, the setup also provides combined usage of the two detectors aligned together to study WAXS and SAXS simultaneously. The setup can be aligned together in the long distance SAXS position (~2.5m) combined with WAXS (27cm) or the intermediate SAXS position (~1.2m) combined with WAXS (27cm).This increases the q range of the WAXS and gives the advantage of simultaneous measurements and reduces exposure time. The combo setup for the intermediate SAXS setup offers q range up to 0.4Å^{-1} for the SAXS and 1.1-4Å^{-1} for WAXS (Figure 5).

Customer testimonial

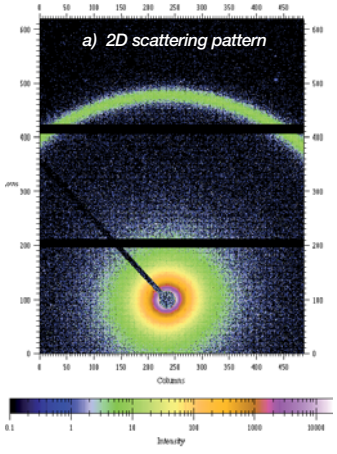
Dr. Roy Beck-Barkai has no financial interests with Xenocs SA products including Genix X-ray Delivering system. Implementation of a SAXS/WAXS combo system with GeniX Low Divergence and scatterless collimation system in Tel-Aviv University is a real success. The system has many big advantages including high flux rate and extreme ease of use. It takes about an hour to completely change configuration hence allows us to conduct many different type of research stimulatingly in the lab.

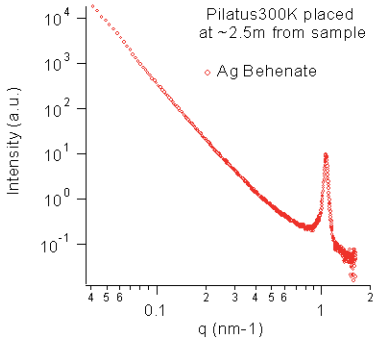
Acknowledgements

Rona Shaharabani and Guy Jacoby are greatly acknowledged for their deep implication in the experimental work.

[i] **Youli Li et al , J. Applied Crystallography (2008) 41, 1134 - 1139**

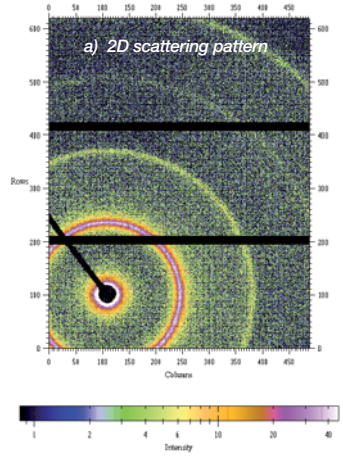
Fig. 2 : Typical SAXS pattern recorded with a Pilatus 300K detector placed at 2.5m from sample.

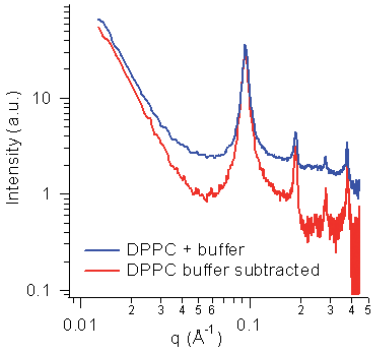




b) Fully azimuthal average of 2D pattern. Q_min better than 4.0e-2 nm-1 enabling probing length scales up to 150nm. Delta Q_detector resolution approx. 2.8e-3 nm-1.

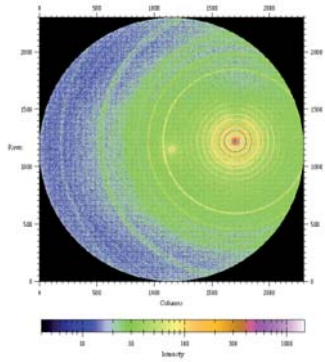
Fig. 3 : Intermediate SAXS pattern of a DPPC 100mmol sample recorded for 30min with a Pilatus 300K detector placed at 1m from sample.





b) Fully azimuthal average of 2D pattern of the sample and of corresponding buffer subtracted data.

Fig. 4: a/ Typical WAXS pattern collected with 2nd detector(MAR345 from Marresearch) placed at approx. 0.27m from sample. Exposure time is 2min. Total air path in air. Point in center of 2D image is a detector artifact. b/ 1D azimuthal averaging of data. 1st order of Ag Behenate at characteristic repeat distance of 5.87nm is clearly detected.



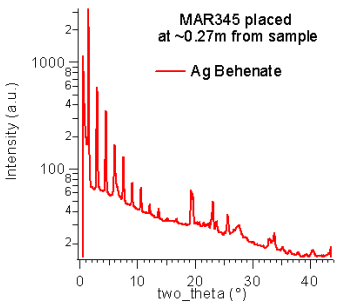
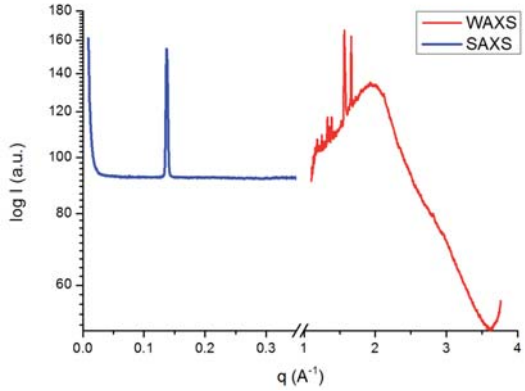


Fig. 5 : SAXS/WAXS combo measurement. 1D azimuthal averaging for the 2D combo SAXS and WAXS images for DLPE (30mg/ml) in HEPES buffer solution. SAXS q range up to 0.35Å^{-1} and for the WAXS 1-4Å^{-1}.



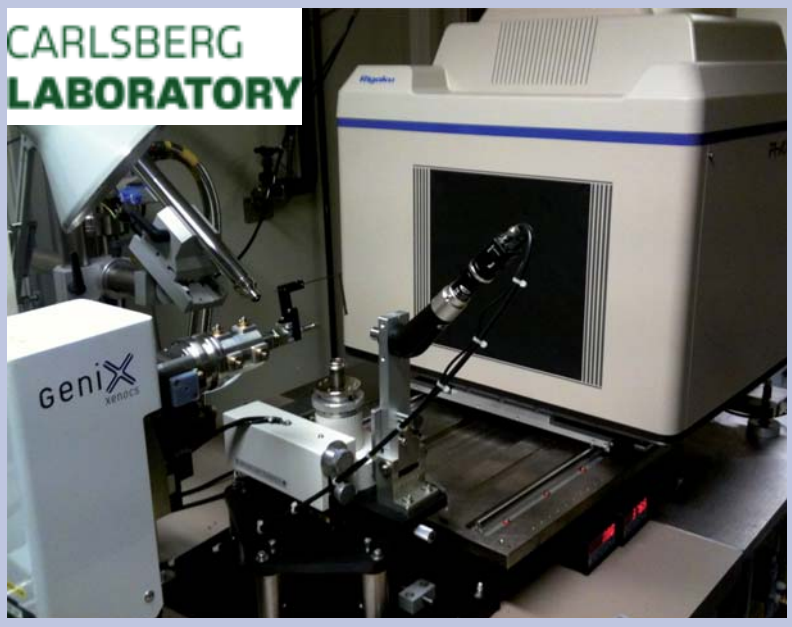


Fig. 6 : X-ray single crystal diffraction equipment at Carlsberg Laboratory

Table 1a and 1b — *Preliminary structure studies of a Human blood group glycosyltransferase mutant to determine the content of the substrate binding site for later soaking experiments.*

Data Courtesy of Dr. René Jorgensen (Protein Chemistry Group)

Table 1a : Crystal parameters

Enzyme	Human blood group glycosyltransferase mutant
Crystal size	200 µm x 100 µm x 500 µm
Space Group	$P2_12_12$
Cell parameters (Å)	52.401 78.038 153.673
Delta phi/image	0.5°
Overall oscillation	135°
Exposure time/frame	5 min

Table 1b : Crystallographic results

Statistics from XDS	Overall	Highest resolution shell
Resolution limits	20 - 2.3 Å	2.4 - 2.3 Å
N. of reflections	128491	12142
N. of unique reflections	27137	2856
Completeness	94.1%	84.4%
Multiplicity	4.5	3.6
Mean ((I)/sd(I))	12.23	3.96
Rmerge	40.9	11.8

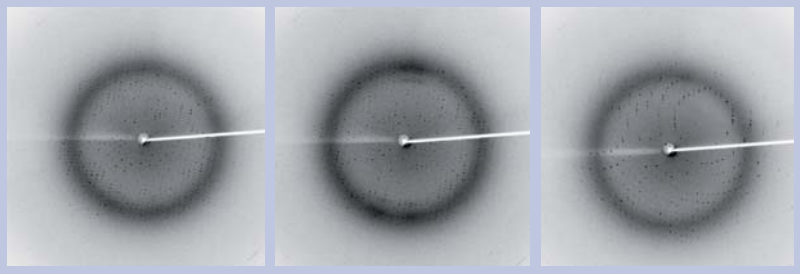


Fig. 2 : Example of diffraction patterns of a human enzyme (see table 1a for crystal parameters)

One year with GeniX at Carlsberg Laboratory

An example of enzyme structural studies preliminary to soaking experiments

In September 2010 a GeniX microsource system has been installed at Carlsberg Laboratory replacing a Rigaku RUH3R rotating anode generator on a protein crystallography set-up. Research at Carlsberg Laboratory employs structural, kinetic and spectroscopic techniques to obtain a detailed molecular description of enzyme reactions. Primary research currently is focused on glycosyltransferases and glycosidases involved in the biosynthesis of oligosaccharides. This includes studying their use in enzymatic synthesis of oligosaccharides, the design and evaluation of glycosyltransferase inhibitors and assay development, including single cell enzymology. This research is part of a major new initiative on structure-function studies on barley starch synthases and detoxification enzymes.

Single crystal diffraction experiments at Carlsberg Laboratory provide static images of the enzymes with different kinds of substrates and inhibitors bound in the active site. This short note and the presented results illustrate the use of a laboratory crystallography set-up based on a low power high brilliance source in a 3D structure analysis of enzymes.

The X-ray equipment at Carlsberg Laboratory is composed of a GeniX Cu HF System (50W, 50 µm Microsource with FOX 3D optics) coupled to a Rigaku R-axis IV++ Image plate detector (see Figure 6). One year after the installation of the GeniX, the X-ray equipment is very frequently used for screening crystal quality and determining suitable cryogenic conditions as well as obtaining space group and unit cell parameters of the crystal. However, occasionally the equipment is also used for collecting entire crystal diffraction data sets to obtain the 3-dimensional structure of the enzymes. An example is illustrated on figure 2 with preliminary structure studies of a human blood group glycosyltransferase mutant.

An X-ray crystallography data set was collected to investigate the state of the enzyme binding site in crystals of the human blood group glycosyltransferase (conditions are summarized in table 1a). A highly redundant data set was recorded (see table 1b).

Often UDP is co-purified with the enzyme. Provided the binding site is empty, other ligand soaking experiments with other crystals from the same crystallization tray could be carry on. The data quality collected with the GeniX was suitable for obtaining a high quality electron density map of the enzymes structure. The result from the solved X-ray structure was that the enzyme molecules in the crystals contained UDP in the binding site. Therefore, is was concluded that in order to perform soaking experiments it is necessary to go through extra measures to remove the UDP from the binding site before crystallizing the enzyme.

Furthermore, in addition to high data quality Dr René Jorgensen seems very satisfied with the low maintenance level of the GeniX. ''**The start up and shutting down of the GeniX seems to be very stable and so far there has been no maintenance on the machine. With the old X-ray generator we had to change the filament every 1-2 months and we are very happy not to have to do this anymore.**''

Xenocs is expanding its worldwide presence

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Since its creation in 2000, Xenocs has been working mostly abroad serving OEM and research groups worldwide. With the active development of its product portfolio, strategic decision has been taken in 2010 to expand the distribution network of the company.

In the beginning of 2011 Xenocs strengthened its position in North and South America by appointing Mosaic Distribution LLC as their new distributor. Mosaic Distribution is well known as distributor in North and South America for Oxford Cryosystems, a world leader in its field, and very complementary to the Xenocs product offerings.

Xenocs has also made its first entry in the Chinese market by signing a strategic distributorship agreement with its long time partner MARresearch. "This agreement is a real opportunity to strengthen our position in China thanks to the synergy of product lines of both companies". Said Hong Wang, MAR Sales Regional Director for China. This agreement is an important step in the development of Xenocs. "This strategic distributorship agreement is a great opportunity for the company. MARresearch is strongly present in China through its local office. This is as well a great evolution of our longtime relationship as Xenocs being supplier of MARresearch" said Frederic Bossan, Marketing&Sales Director of Xenocs.

Xenocs has organized in early 2011 its annual distributor seminar which was a great occasion for all the team of distributors to meet, share experiences and get updated on the latest evolution of our product portfolio. "I was thrilled to meet the Xenocs team, and learn more about the technical excellence of Xenocs products and level of expertise of the team" said Liz Carter, President of Mosaic Distribution.

This seminar was done partly at Xenocs and partly at our application lab at the European Molecular Biology Laboratory (EMBL) for full training of our distributor team on installation and maintenance of our product range. "This seminar was a great occasion to learn all the details of installation and maintenance procedures of the new Xenocs products" said Suresh Pemmaiah, President of HP Instruments, distributor of Xenocs for India.

Specific training sessions have been done at Chamonix on our newly available SAXS system product range so our team of distributors has complete understanding of the concept, key customer benefits, and performance attributes for the product range. "These SAXS cessions organized by Dr. Panine, application scientist at Xenocs and 10 year research scientist at ESRF, was a great occasion to learn more about Xenocs SAXS system product line, and its unique advantages", said Xiao ZHANG, sales manager at MAR China Office.

Having such a dynamic team of distributors is a real asset for the company, said Frederic Bossan, we consider them as complete part of the Xenocs team. We work in close collaboration with them in order to give the best level of advice and support to our customers.

Xenocs will continue to expand its distribution network to other demanding regions in order to continuously better serve its customers.

Forthcoming Conferences 2012

Jan 18-19, Göteborg, SWEDEN
NSSM 2012
9th Nordic Workshop on Scattering from Soft Matter

Mar 12-15, Munich, Germany
DGK 2012
German Society for Crystallography

Apr 16-19, Warwick University, UK
BCA
BCA Spring Meeting

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A spin-off company from Institut Laue Langevin