**Appendix A**

Description of the Subject of Public Procurement

**Part 1:**

Hybrid Photon Counting detector for macromolecular crystallography for SOLCRYS beamline at SOLARIS NSRC

**Part 2:**

Synchrotron microdiffractometer for protein crystallography for SOLCRYS beamline at SOLARIS NSRC

[**Part 1**: 3](#_Toc199507581)

[1. General information 3](#_Toc199507582)

[2. General specification of the scope of delivery 3](#_Toc199507583)

[2.1. Detector technical specification 4](#_Toc199507584)

[2.2. Control unit 5](#_Toc199507585)

[2.3. Thermal stabilization unit 5](#_Toc199507586)

[3. Additional information 5](#_Toc199507587)

[**Part 2**: 6](#_Toc199507588)

[1. General information 6](#_Toc199507589)

[2. General specification of the scope of delivery 6](#_Toc199507590)

[2.1. Sample positioning axes 7](#_Toc199507591)

[2.2. X-ray beam conditioning 8](#_Toc199507592)

[2.3. Sample visualization 10](#_Toc199507593)

[2.3.1. On-axis video microscope 10](#_Toc199507594)

[2.3.2. Backlight system 10](#_Toc199507595)

[2.3.3. Frontlight system 10](#_Toc199507596)

[2.4. Kappa goniometer head 10](#_Toc199507597)

[2.5. Support mechanism for diamond anvil cell 10](#_Toc199507598)

[2.6. Fluorescence detector table 11](#_Toc199507599)

[2.7. X-ray shutter 11](#_Toc199507600)

[2.8. Interface box 11](#_Toc199507601)

[2.9. Alignment laser 11](#_Toc199507602)

[2.10. Control 11](#_Toc199507603)

[3. Additional conditions – applies to part 2 12](#_Toc199507604)

[3.1. Final design 12](#_Toc199507605)

[3.2. Delivery, installation and Site Acceptance Tests 12](#_Toc199507606)

[**Appendices 13**](#_Toc199507607)

# **Part 1**:

# General information

The objective of this tender is the manufacturing, delivery and installation of Hybrid Photon Counting detector for macromolecular X-ray crystallography. The device will be installed at a SOLCRYS (ARYA) beamline at SOLARIS National Synchrotron Radiation Centre in Krakow, Poland.

The SOLCRYS beamline is designed for macromolecular crystallography (MX) using synchrotron radiation in the energy range from 4 to 22 keV. The expected research capabilities of the MX end station include tunable radiation wavelength for multi-wavelength anomalous diffraction (MAD) experiments and high-flux mode for standard (routine) diffraction data collection on protein crystals. Expected technical parameters of the beamline are presented in Table 1.

**Table 1. Expected technical parameters of the SOLCRYS beamline.**

|  |  |
| --- | --- |
| Energy range | 4-22 keV |
| Beam size at a sample | 260 x 80 µm |
| High resolution mode  - flux at 12 keV - energy resolution | ~1012 ph/s 1.4x10-4 (ΔE/E) |
| High flux mode - flux at 12 keV - energy resolution | ~1013 ph/s  0.5-1% (ΔE/E) |
| Divergence | 1.9 mrad x 0.3 mrad |
| Position of a sample | 42 m from source |

# General specification of the scope of delivery

The Contractor shall manufacture, deliver and install a fully functional detector designed for macromolecular X-ray crystallography experiments to be conducted at a synchrotron beamline. The detector must be designed to capture X-ray diffraction patterns with exceptional speed and accuracy, providing critical data for determining the atomic structure of large biological macromolecules like proteins and nucleic acids. The detector needs to have high active area, high framerate, high dynamic range and low background noise. The detector must be fully compatible with standard protein crystallography beamline infrastructure and must also be fully interoperable with the MXCuBE software, which will be used for experiment control and data acquisition. Detector will be installed on the beamline prior to installation of the X-ray optics system.

The detailed technical specification is described in sections below.

## Detector technical specification

Detector’s high-speed and high-resolution capabilities should allow for fast and precise data collection from macromolecular crystals at synchrotron beamline. It should be compatible with different modes of data collection, such as standard collection, fine slicing, radiation damage studies and studies using Diamond Anvil Cells. The required technical specifications are:

* Detector technology: Hybrid Photon Counting (HPC)
* Number of modules (W x H): not less than 3 x 6 = 18
* Sensor material: Silicon (Si)
* Sensor thickness: not more than 450 µm
* Pixel size (W x H): not bigger than 75 µm x 75 µm = 5625 µm2
* Pixel array format (W x H): not less than 3108 pixel x 3262 pixel = 10 138 296 pixel
* Active area (W x H): not less than 233.1 mm x 244.65 mm = 57 027.915 mm2
* Inter-module gap: not more than hor. 12 pixels, vert. 38 pixels
* Defective pixels: less than 0.05%
* Image bit depth: 32 ,16 or 8 bit
* Readout bit depth 16 or 8 bit
* Maximum count rate: not less than 1.7 × 109 photons/s/mm2
* Adjustable threshold range: not worse than 3.5 keV to 30 keV
* Energy range: not worse than 6 keV to 22 keV
* Number of thresholds: at least two independent thresholds
* Readout time: continuous readout with not more than 100 ns dead time
* Maximum frame rate (continuous): not worse than 490 Hz (8 bit), 245 Hz (16 bit)
* ROI maximum frame rate (continuous): not worse than 1120 Hz (8 bit), 560 Hz (16 bit)
* Point-spread function: 1 pixel (FWHM)

## Control unit

The detector must be equipped with the control unit that serves as the interface between the detector and the rest of the experimental setup, controlling and managing all aspects of the detector’s operation. The details of the control unit are left to the contractor. Parameters of the control unit have to be included in the offer.

## Thermal stabilization unit

The detector must be equipped with the thermal stabilization unit. The details of the chiller are left to the Contractor. Parameters of the chiller must be included in the offer.

# Additional information

The offer must include a concept of the detector, chiller and control unit. Delivery of the Subject of the Order specified for part 1 will take place in accordance with the attached contract template. For the on-site installation and testing, it is expected the presence of at least one specialized person for minimum 1 working day. The detector will be installed on a dedicated detector support table, which is the subject of another tender. Details regarding the table will be provided to the Contractor after the tender for the experimental tables is resolved.

# **Part 2**:

# General information

The object matter of the order is the design, manufacturing, delivery and installation of a high- precision diffractometer for macromolecular X-ray crystallography. The device will be installed in a SOLCRYS (ARYA) beamline at SOLARIS National Synchrotron Radiation Centre in Krakow, Poland.

The SOLCRYS beamline is designed for macromolecular crystallography (MX) using synchrotron radiation in the energy range from 4 to 22 keV. The expected research capabilities of the MX end station include tunable radiation wavelength for multi-wavelength anomalous diffraction (MAD) experiments and high-flux mode for standard (routine) diffraction data collection on protein crystals. Expected technical parameters of the beamline are presented in Table 1.

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| Divergence | 1.9 mrad x 0.3 mrad |
| Position of a sample | 42 m from source |

# General specification of the scope of delivery

The Contractor must manufacture, test, deliver and install a fully operational microdiffractometer specifically designed for macromolecular X-ray crystallography experiments to be conducted at a synchrotron beamline. The microdiffractometer must be capable of performing high-precision crystallographic diffraction data measurements with exceptional accuracy, suitable for single-crystal analysis. The system must support multiple data collection modes, including: standard, helical, grid, and raster scanning techniques, as well as experiments utilizing Merrill-Bassett Diamond Anvil Cells (DACs). The equipment has to be be optimized to facilitate flexible, high-throughput data acquisition under various experimental conditions.

Additionally, the microdiffractometer must be fully compatible with standard protein crystallography beamline infrastructure. This includes, but is not limited to, integration with a sample-changing robot (e.g., Irelec or equivalent), detectors such as Dectris EIGER2 (or similar high-performance detectors), and a fluorescence detector. Compatibility with cryostream systems for cryogenic cooling of samples is also required.

The system must also be fully interoperable with the MXCuBE software, which will be used for experiment control and data acquisition. The Contractor must ensure that all necessary drivers, software modules, and interfaces are provided to enable seamless integration with MXCuBE, allowing for efficient experiment setup, monitoring, and data collection.

The Contractor is required to follow the requirements and standards, describing technologies and materials used in SOLARIS. All of the requirements are described in Appendices listed in section 4.

The detailed specifications of the diffractometer is described in following paragraphs.

## Sample positioning axes

The microdiffractometer must support a variety of movements for sample centering and data collection, including but not limited to: omega rotation, alignment (AX), raster and grid scans (AY, AZ), centering, and helical scans (CX, XY). These movements should be fully controllable with high precision to facilitate accurate and reliable data acquisition. Detailed specifications and requirements for each axis of movement are provided in Table 2. The orientation of Ω axis should be vertical.

Table 2. Minimal requirements for sample positioning axes

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | *max. Speed* | *SOC radius* | *Range* | *Resolution* | *Dynamic accuracy* | *Repeatability* |
| **Ω** | not less than 720 deg/s | ≤200 nm at 10 deg/s | no limit | not worse than 0.1 µdeg | below ± mdeg at 10 deg/s | better than ± 0.5 mdeg |
| **AX** | not less than 2 mm/s | - | ≥5 mm | not worse than 16 nm | not specified | better than ± 2 µm |
| **AY** | not less than 15 mm/s | - | ≥108 mm | not worse than 10 nm | below 1 µm at 15 mm/s on load | better than ±150 nm on load |
| **AZ** | not less than 3 mm/s | - | ≥6 mm | not worse than 16 nm | not specified | better than ± 2 µm |
| **CX** | ≥1 mm/s | - | ≥6 mm | not worse than 10 nm | below ± 1µm at 1 mm/s on load | better than ±100 nm on load |
| **CY** | ≥1 mm/s | - | ≥6 mm | not worse than 10 nm | below ± 1µm at 1 mm/s on load | better than ±100 nm on load |

## X-ray beam conditioning

The microdiffractometer must be capable of focusing X-rays to a spot size within a range of approximately 10 to 200 microns, offering sufficient flexibility to accommodate a broad spectrum of sample sizes and experimental configurations. The system shall be equipped with a minimum of five (5) beam apertures, each supported by a precise control mechanism that allows for seamless and high-accuracy switching between apertures. The detailed specifications for the aperture diameters, as well as the associated control systems, shall be finalized and agreed upon during the Final Design Review (FDR).

The diffractometer must be equipped with a **movable capillary system**, complete with a support blade and scatter guard, ensuring secure and stable positioning of samples while minimizing background noise from scattered radiation. It is expected that at least one spare capillary will be included.

Additionally, the diffractometer must include a **scintillator unit** mounted on an XYZ table. The X-axis of the scintillator unit should be mechanically coupled with the X-axis of the beamstop to ensure precise alignment and movement. The scintillator unit shall comprise a **CWO crystal and a pin diode for** optimal X-ray light conversion and signal detection.

The **beamstop unit** must be motorized, offering precise control for positioning and adjustments during data collection. It is expected that two different beamstops will be included in the offer.

The detailed requirements for all beam conditioning unit movements, including the capillary, scintillator, and beamstop, are summarized in Table 3.

Table 3. Minimal requirements for beam conditioning unit movements.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | *Motor type* | *Max Speed* | *Range* | *Encoder type* | *Resolution* | *Repeatability* |
| **Apperture Y (side)** | DC | ≥ 2 mm/s | ≥ 4 mm | Circular encoder on motor unit | ≥ 16 nm (60620.8 cts/mm) | ≥ ±1 µm |
| **Apperture Z (in-out)** | DC | ≥ 4 mm/s | ≥97 mm | Circular encoder on motor unit | ≥45 nm (22300 cts/mm) | ≥ ±1 µm |
| **Capillary Y (side)** | DC | ≥ 2 mm/s | ≥ 2 mm | Circular encoder on motor unit | ≥ 16 nm (60620.8 cts/mm) | ≥ ±2 µm |
| **Capillary Z**  **(in-out)** | DC | ≥ 20 mm/s | ≥97 mm | Circular encoder on motor unit | ≥ 90 nm (11150 cts/mm) | ≥ ±2 µm |
| **Scintillator (in-out)** | DC | ≥ 20 mm/s | ≥97 mm | Circular encoder on motor unit | ≥ 90 nm (11150 cts/mm) | ≥ ±2 µm |
| **Beamstop X (along X-rays)** | DC | ≥ 20 mm/s | ≥52 ±1 mm | - | ≥ 90 nm (11150 cts/mm) | ≥ ±2 µm |
| **Beamstop Y (side)** | DC | ≥ 2 mm/s | ≥ 4 mm | - | ≥ 16 nm (60620.8 cts/mm) | ≥ ±2 µm |
| **Beamstop Z (in-out)** | DC | ≥ 20 mm/s | ≥97 mm | - | ≥45 nm (22300 cts/mm) | ≥ ±2 µm |

## Sample visualization

The microdiffractometer must be equipped with light systems and on-axis video microscope for sample visualization and centering. The details will be described in following sections.

## 2.3.1. On-axis video microscope

The microdiffractometer must be equipped with on-axis video microscope with digital high resolution cameras. The magnification should be at least in the range of x2.5 to x30. The access to all zoom levels should be instant. The software needs to be fully integrated with high speed image server for multiple image distribution.

## 2.3.2. Backlight system

The system must be equipped with integrated backlight system with transmitted lighting. The optical fiber guide of length 5 m should be included.

## 2.3.3. Frontlight system

The system must be equipped with reflected lightning – frontlight system with two light sources working in reflection. Two optical fiber guides of length 5 m each should be included – one for each light source. The light sources should be mounted to objective head of on-axis video microscope.

## Kappa goniometer head

The diffractometer must be equipped with kappa goniometer head compatible with the centering stage. The mounting of the head should allow fast and simple head replacement. The head should be automatically recognized by the system by individual digital code or other solution. The goniometer head should be adapted for magnetic mounting of samples on SPINE and miniSPINE holders.

## Support mechanism for diamond anvil cell

The diffractometer must be equipped with additional goniometer head dedicated to experiments with diamond anvil cells. The mounting of the head should allow fast and simple head replacement. The head should be automatically recognized by the system by individual digital code or other solution. The details of mounting the DAC on the goniometer head are left to the Contractor and should be presented in Preliminary Design Review stage of the Contract.

## Fluorescence detector table

The system must be equipped with fluorescence detector table, pneumatically retracted. The table should be adapted to a specific detector model. Details about the detector will be provided to the contractor at the design stage. Fluorescence detector should be fully integrated with software and allow the remote control and interlock handling.

## X-ray shutter

The system must be equipped with the fast X-ray shutter with frictionless mechanics and should be mounted to the diffractometer assembly frame. The electronics of the shutter should be integrated into diffractometer rack.

## Interface box

The offer must include the interface electronics for sample changer robot. The exact model of the robot will be specified at the Preliminary Design stage of the contract. Interface box must allow matching the sample changer robot signals with diffractometer control signals and allow the synchronization between sample changing robot, cryo-retraction table and shutter.

## Alignment laser

For the alignment purposes, it is necessary to equip the system with the green alignment laser for alignment purposes without x-rays. The alignment laser should allow the manual co-axial alignment with 5 degrees of freedom (x, y, z, pitch, yaw). The laser must have the possibility to be mounted on the frame of microdiffractometer.

## Control

The Contractor is required to follow the technological requirements described in Control System Standard for New Accelerator, Front End and Beamline Components (see Appendix CS0) and in Motion Control Standard (see Appendix CS1). The embedded control parameters are described in Table 4.

Table 4. Embedded Control parameters.

|  |  |
| --- | --- |
| Technology | PowerBrick including new generation amplifiers |
| CPU | 1 GHz |
| Ethernet | 1 GB/s |

# 3. Additional conditions – applies to part 2

## Final design

The Ordering Party require the Contractor to submit a preliminary design report (PDR) and next a final design report (FDR). The Ordering Party require that the final design will be presented by the Contractor no later than 8 weeks upon signing the contract.

The final project should include at least the following:

* 2D and 3D drawings (STEP)
* List of all components for delivery
* Types of motors with encoders and connection diagram
* Parameters of motor movements (see Appendix CS1)
* Description of testing procedure (FAT and SAT)
* Transport and unpacking instructions
* Manual movements and transport instructions

## Delivery, installation and Site Acceptance Tests

Delivery of the Subject of the Order specified for part 2 will take place in accordance with the attached contract template. For the on-site installation and testing, it is expected the presence of two specialized persons for 2 weeks (10 working days). The diffractometer will be installed on a dedicated diffractometer support table, which is the subject of another tender. Details regarding the table will be provided to the Contractor after the tender for the experimental tables is resolved.

# Appendices

The reference documents are appended with the following attachments. The Attachments include technological descriptions used in SOLARIS, which the Contractor shall observe and comply with. Attachments constitute an integral part of the Terms of Reference.

1. Appendix ALIGN - Guidelines in field of alignment
2. Appendix CS0-SOLARIS Control System Standard
3. Appendix CS1 - Motion Control Standard
4. Appendix CS2 - Detailed responsibility matrix for Control System tasks
5. Appendix CS3 – Standard elements
6. Appendix MECH1 – Mechanics
7. Appendix MECH 3 - Description of the ID03 Beamline area
8. Appendix MECH 4 - Dimensions of the ID03 Beamline area
9. Appendix SOURCE - synchrotron radiation source parameters
10. Appendix SOURCE-ID03 3-pole wiggler parameters
11. Appendix WAT-CA1 compressed air basic standards\_2.2
12. Appendix WAT-CW1 cooling water basic standards\_2.2