

XtalTool

Sample Holder for Crystal Growth, *in situ* Ligand Soaking and Data Collection

Cat. No.	Amount
X-XT-101	24 XtalTool Sample Holder 1 Customized Goniometer Base (Type B5)

Application

Sample holder for crystal growth, soaking and X-ray data collection without the need of direct crystal manipulation or mounting^[1].

Kit Contents

24 XtalTool Sample Holder
1 Customized Goniometer Base (Type B5)

Description

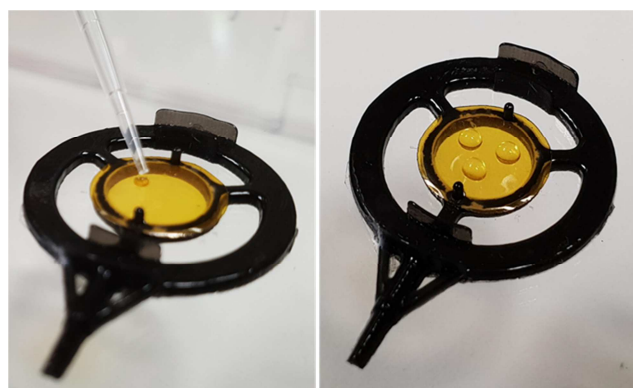
The XtalTool is a patent-pending^[2] 22 mm sample holder consisting of a plastic support with an outer transparent COC film and an inner X-ray transparent yellow polyimide film with 5 µm pores. The design allows the setup of multiple crystallization drops and does not compromise the monitoring of crystals under the microscope. Mounted on the supplied goniometer base it meets the 18 mm SPINE standard and is compatible with most synchrotron and in-house beamlines.

The XtalTool enables crystal growth, manipulation and X-ray data collection at room and cryogenic temperature, all in one.

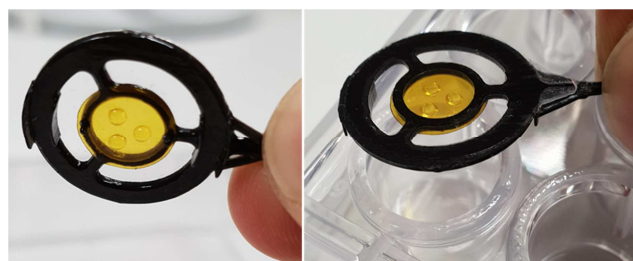
Usage

*Note: **Do not touch** the yellow foil with unprotected fingers to avoid contamination. The usage of protected forceps is recommended.*

1. Take one XtalTool from its box and place it with the outer transparent film on a smooth surface to avoid damage and unwanted puncture of the film. Setup your crystallization drops on the yellow polyimide film, as you would do on a regular cover slide. Do not pierce the film.



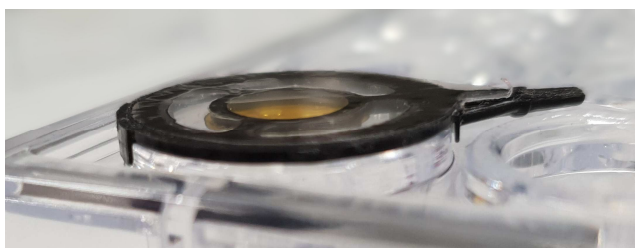
2. Flip over the sample holder and place it onto a greased cavity of a 24 well plate. The design is such that 24 sample holders will fit a 24 well plate.



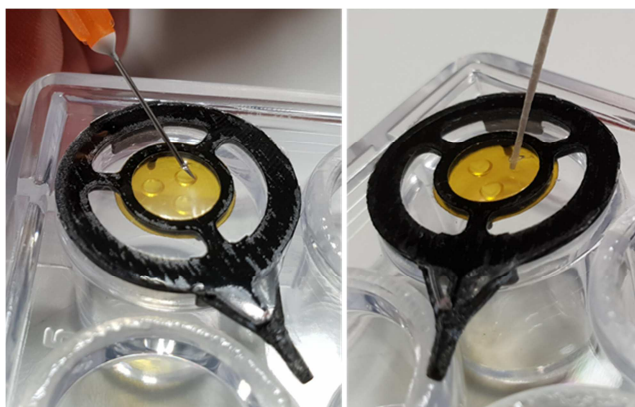
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- Seal the cavity with the sample holder. Ensure that XtalTool is placed correctly as indicated by the two ears on either side.



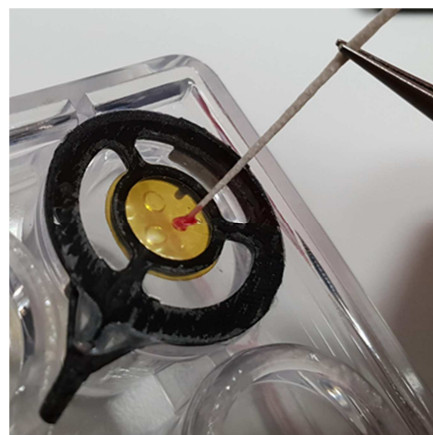
- Ligand soaking: Remove mother liquor in a two-step procedure:
 - First, carefully poke a hole into the upper COC film at the appropriate position using a fine needle. The position of the puncture should be right next to the desired drop.
 - Second, insert a fine paper wick into the poked hole and carefully push it down until it gently touches the polyimide film. Keep the paper in contact with the perforated film to absorb the liquid. The required time highly depends on the viscosity of the mother liquor composition. Once done, gently retract the paper wick.



Now gently insert a long tip and apply a small volume of a ligand mother liquor solution adjacent to the crystal. Efficient soaking is achieved by placing the drop as accurately as possible. Do not puncture the yellow film. Retract the tip and gently touch the film with protected warm finger for 2 seconds and slide across, the film will reseal itself.



The applied solution will diffuse through the micro pores to the crystal growing side. Incubate the plate for a desired soaking time and remove the excess soaking solution with a new fine paper wick. You may soak with different compounds subsequently.



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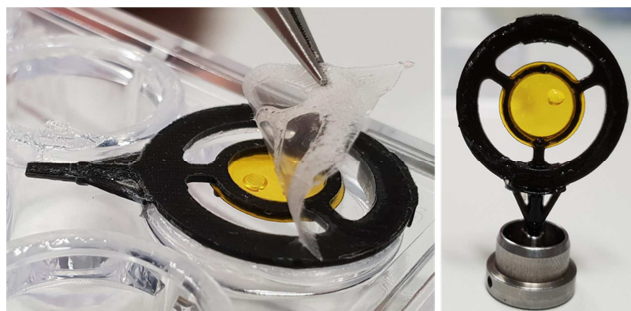
Note 1: Suitable material for crystal soaking on an XtalTool is provided in the XtalTool Soaking Kit (Cat. No. X-XT-102).

Note 2: The ligand containing solution can also be applied without prior removal of the mother liquor solution. This setup allows for more gentle soaking conditions where the high ligand concentration slowly exchanges. Hence, soaking time needs to be extended and adjusted accordingly.

- Crystal cryo-protection: Apply the cryo solution in the gap between the outer COC and the inner polyimide film. After the desired incubation time, remove the solution with a fine paper wick. The time to attain cryo-protected crystals is highly dependent on the employed components.

Note: The removal of mother liquor and/or cryo solution before data collection is recommended to minimize solvent scattering. If diffraction data are collected at ambient temperature, residual mother liquor solution can also be removed using a paper wick within the humidity on the goniometer.

- X-ray data collection: Gently remove the transparent COC back film. Still existing mother liquor and/or cryo solution can now be efficiently removed using a paper wick. Mount the sample holder on a goniometer via the supplied customized base. If data collection at cryogenic temperature is desired, mounting without direct cryo-stream is recommended. The mounted sample holder is then flash frozen using the cryo stream.



Note: The removal of mother liquor may not be necessary when data is collected at ambient temperature. Yet, it is recommended to prevent crystal displacement, which can occur in the excess solution during data collection.

The XtalTool was developed by the HZB MX-group at BESSY II (AG Weiss).

Related Products

- 24 Well SuperClear Plates (Cat. No. CPL-130, CPL-132)
- XtalTool Soaking Kit (Cat. No. X-XT-102)
- XtalTool HT (Cat. No. X-XT-103, X-XT-104)

References

- [1] Feiler *et al.* (2019) An All-in-one Sample Holder for Macromolecular X-ray Crystallography with Minimal Background Scattering. *J. Vis. Exp.* **149**:e59722.
- [2] XtalTool: Patent DE 10 2017 129 761.8, Christian G. Feiler, Dirk Wallacher, Manfred S. Weiss, filing date: 13.12.2017, An international patent application via the PCT route, WO 2019114879 A1 using the priority of DE 10 2017 129 761.8 has been filed, PCT/DE2018/101007.