

ESRF	Experiment title: Structural study on PatAB multidrug ABCtransporter	Experiment number: MX-2441
Beamline:	Date of experiment:	Date of report:
CM01	from: 10/07/2023 to: 12/07/2023	30/08/2023
Shifts:	Local contact(s): Eaazhisai KANDIAH	Received at ESRF:
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Report:

We have applied for time on the Titan KRIOS (CM01) as a member of the France BAG (MX2441) coordinated by Laurent TERRADOT. The propose is to get structural information on PatAB a heterodimer ABC transporter Multidrug involved in the resistance to fluoroquinolones. We study the intricate molecular mechanism (spectrum of drug recognition, nucleotide hydrolysis mechanism of this transporter. Its functions according to an asymmetric catalytic cycle, remains obscure because its two nucleotide-binding sites are non-equivalent.

The session was scheduled on 10th July and data were collected remotely. Three home-screened grids (quantifoil R1.2/1.3 Au 200 mesh) were sent to ESRF. A multi-grid session was performed on two grids of the sample prepared into two different buffers. The session was finished Wednesday 12th morning.

12134 micrographs were collected on the first grid and 16534 on the second grid. The ESRF processing pipeline indicates that the majority of micrograph has a resolution below 3 ang. And 2D classification performed on a small set of particles shows 2D classes with very nice details (figure1).



Figure 1 : Several 2D classes extracted from 2D classification preformed a small data set (from ESRFprocessing pipeline)

The file transfer from ESRF to our server took more than two weeks. We have currently starting to process the data. Based on the quality of the ESRF processing, we expected very good 2D classes and 3D reconstruction with a high resolution. The report will be updated once we perform full data processing.