	Experiment title: Characterization of ABC transporter conformational changes.	**Experiment number**: MX-2441
Beamline: CM01	**Date of experiment**: from: 17/03/23 to: 19/03/23	**Date of report**: 21/08/23
Shifts: 6	**Local contact(s)**: Gregory Effantin	*Received at ESRF:*

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Report:

We benefitted from 6 shifts that we have split in 2 data collection sections. The whole data collection was a success.

- **The multidrug resistance ABC transporter Cdr1 from C. glabrata**.

We have collected around 10,000 movies, that yielded many wonderful results .We were first able to get a structure of the transporter at 2.8Å resolution, in a post catalytic state in complex with ADP-Vanadate. This allowed for a detailed model building with unambiguous density and placing for side chains.

In addition, on the same grid, we were able to obtain the next wtructure with departure of Vanadate, with only ADP remaining, at 3.2 Å resolution. This shows outstanding helical deformations, and rearrangements of the trasnporter linked to vanadate/phosphate release, which is an essential step of the return of the transproter to the inward-facing conformation and reset for another transport cycle.

Moreover, using inter-particle variability calculated using 3DVA (that we have greatly optimized to visualize movements), we were able to capture the whole conformational change of the transporter. These results, highlight the pasticity of the transporter and reveals key deformation hotspots on the structure, as well as the

role of cofactors in stabilizing parts of the structure. These results are currently being formatted for publication.

- **Time-resolved cryoEM characterization of the inward->outward conformatinal change for the ABC transporter BmrA from B. subtilis.**

For this transporter, we have already collected many structures and have the full steady-state view of the transporter and conformational changes. We are now interested in gaining time-resolved dynamics of these changes. We have characterized the biochemical parameters to control the transition, which allwed us to slow down the process. We have already collected the first 2 time-points, this collection was for the last third time-point. Data processing is under way, but we can already say that it worked well, and gives us good reconstructions, in-line with our biochemical data. In addition, we have visualized interesting, new, conformational changes linked with the transporter's fonction. These data will be formatted for publication in a near future.