

Oral presentation

Serial crystallography at PETRA III beamline P11

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P11 at PETRA III (DESY, Hamburg) is a high-throughput instrument for macromolecular crystallography [1]. P11 has tuneable photon energy between 5.5 - 28 keV having the Eiger2 X 16M as the stationary detector. Beam size from 200x200 μm^2 to 4x9 μm^2 can be used with a maximum photon flux of 1×10^{13} ph/s at 12 keV energy.

P11 is a diverse environment able to accommodate various non-standard experiments. For example, serial synchrotron crystallography (SSX) is enabled with sample delivery through various types of solid supports and the TapeDrive setup (Fig. 1), which allows time-resolved room temperature experiments by the mix-and-diffuse method [2], and has been developed at P11 along with the real-time autoprocessing with CrystFEL [3, 4]. In this method sample is delivered on to a continuously drawn polyimide tape through a 3D-printed microfluidic nozzle with two channels (\varnothing 150 μm each), one for the crystal slurry and second, for example, for mixing the crystals with a ligand or adjusting their pH. The mixing time can be modified by the speed of the tape and the distance of the nozzle from the X-ray focus point (delay times of 50 ms – 180 s). The effects of temperature can be studied using a separate gas nozzle for sample heating. Furthermore, exposure time can be controlled with a rotating chopper wheel. Through combination of these parameters multidimensional SSX experiments are enabled. TapeDrive is currently controlled through a separate graphical user interface, and online data analysis is available for real-time evaluation and indexing via OnDA Monitor [5].

P11 is in the process of employing MXCuBE as the default data acquisition software with the integration to ISPyB for tracking shipments, communicating the sample details to MXCuBE, as well as acting as a data archive and presenting preliminary data processing results. These will be expanded to be used with the SSX experiments, too. These developments are synchronising P11 with the EMBL PETRA III beamlines for the future foundation of a uniform structural biology village at PETRA IV.

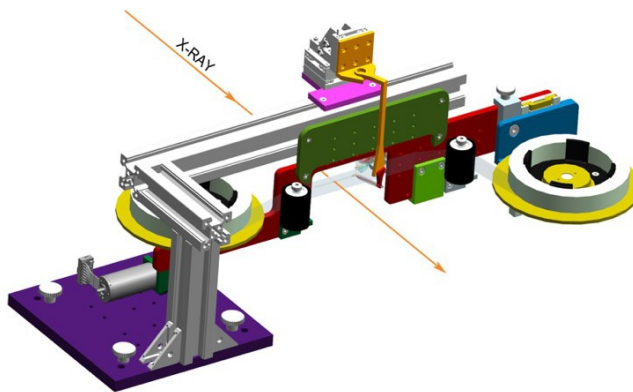


Figure 1. CFEL TapeDrive, a conveyor belt-based sample delivery system for multi-dimensional serial crystallography.

- [1] Burkhardt, A., Pakendorf, T., Reime, B., Meyer, J., Fischer, P., Stübe, N., Panneerselvam, S., Lorbeer, O., Stachnik, K., Warner, M., Rödiger, P., Göries, D. & Meents, A. (2016). *Eur. Phys. J. Plus* **131**, 56.
- [2] Beyerlein, K. R., Dierksmeyer, D., Mariani, V., Kuhn, M., Sarrou, I., Ottaviano, A., Awel, S., Knoska, J., Fuglerud, S., Jönsson, O., Stern, S., Wiedorn, M. O., Yefanov, O., Adriano, L., Bean, R., Burkhardt, A., Fischer, P., Heymann, M., Horke, D. A., Jungnickel, K. E. J., Kovaleva, E., Lorbeer, O., Metz, M., Meyer, J., Morgan, A., Pande, K., Panneerselvam, S., Seuring, C., Tolstikova, A., Lieske, J., Aplin, S., Roessle, M., White, T. A., Chapman, H. N., Meents, A. & Oberthür, D. (2017). *IUCrJ* **4**, 769.
- [3] White, T. A., Mariani, V., Brehm, W., Yefanov, O., Barty, A., Beyerlein, K. R., Chervinskii, F., Galli, L., Gati, C., Nakane, T., Tolstikova, A., Yamashita, K., Yoon, C. H., Diederichs, K. & Chapman, H. N. (2016). *J. Appl. Cryst.* **49**, 680.
- [4] White, T. A., Schoof, T., Yakubov, S., Tolstikova, A., Middendorf, P., Karneviskiy, M., Mariani, V., Henkel, A., Klopprogge, B., Hannappel, J., Oberthür, D., De Gennaro Aquino, I., Egorov, D., Munke, A., Sprenger, J., Pompidor, G., Taberman, H., Gruzinov, A., Meyer, J., Hakanpää, J., & Gasthuber, G. (2024). *IUCrJ* In review.
- [5] Mariani, V., Morgan, A., Yoon, C. H., Lane, T. J., White, T. A., O'Grady, C., Kuhn, M., Aplin, S., Koglin, J., Barty, A. & Chapman, H. N. (2016). *J. Appl. Cryst.* **49**, 1073.