MS2-04 **Humidity controlled Protein Powder Diffraction, application on an urchin-like polycrystal of the Mayaro virus nsp3 macrodomain.** Yves Watier[a], Nicolas Papageorgiou,[b] Coutard Bruno,[b] Lantez Violaine,[b] Gould Ernest A.,[b] Fitch Andrew N.,[a] Wright Jonathan P.,[a] Canard Bruno,[b] Margiolaki Irene,[c] *[a]European Synchrotron Radiation Facility, ESRF, BP-220, 38043 Grenoble, FRANCE, [b]Architecture et Fonction des Macromolécules Biologiques, CNRS and Universités d'Aix-Marseille I et II, UMR 6098, ESIL Case 925, 13288 Marseille, FRANCE, [c] Department of Biology, Section of Genetics, Cell Biology and Development, University of Patras, GRECE*
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Protein powder diffraction on small amount of sample, as typically found in crystallisation drops used to be challenging. The capillary, routinely used in powder diffraction shown to be problematic with protein polycrystals. When the crystals are not robust enough they do not survive the centrifuging inside a capillary. Here we present a method to collect at room temperature on a typical PX beamline a powder diffraction pattern keeping the sample from dehydrating via a humidity control device available at the ESRF.

A test case using glucose isomerase microcrystals shown the possibility to obtain sufficient informations to redetermine the structure using molecular replacement.

We will present the sample preparation, data acquisition and results obtained on the non structural protein 3 macrodomain of the Mayaro virus, collected ar ID14 using only a single urchin-like crystal, at room temperature under humidity control, following previous studies[1].

[1] Papageorgiou, N. and Watier, Y. and Saunders, L. and Coutard, B. and Lantez, V. and Gould, E.A. and Fitch, A.N. and Wright, J.P. and Canard, B. and Margiolaki, I. Preliminary insights into the non structural protein 3 macro domain of the Mayaro virus by powder diffraction Z. Kristallogr 2010, 225, 576-580

Keywords: protein, powder, virus

MS2-05 **Improvement of the diffraction quality of macromolecular crystals at European synchrotrons using the HC1 dehydration control device** Uwe Mueller[a], Manfred S. Weiss [a], Juan Sanchez-Weatherby[b], Thomas L-M. Sorensen[b], Marjolein Thunnissen[c], Thomas Ursby[c], Alexandre Gobbo [d], Silvia Russi [d], Matthew W. Bowler [d]and Florent Cipriani [d] *[a]Helmholtz-Zentrum Berlin, F-I2, Macromolecular Crystallography (HZB-MX), Albert-Einstein-Str. 15, 12489 Berlin,Germany, [b]Diamond Light Source Ltd. Harwell Science and Innovation Campus RAL, Chilton, Didcot, Oxfordshire, OX11 0DE, United Kingdom [c]MAX IV Laboratory, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden [d]EMBL Grenoble, 6 Rue Jules Horowitz,BP 181, 38042 Grenoble CEDEX 9, France*
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The availability of high quality X-ray diffraction data is needed to answer important questions concerning the structure-function relationship of biological macromolecules. Such data can only be obtained if well diffracting single crystals of the proteins or complexes between proteins and other molecules are available. However, many crystals do not meet these requirements and it can often be difficult to modify them so that they attain the desired properties.

The controlled dehydration of crystals is a method, which can be regarded as an additional optimization path for the improvement of the diffraction quality of many macromolecular crystals, including membrane proteins [1-4]. In addition it also supplies a method to investigate the effect of cryo-cooling and the choice of cryo-protectant more thoroughly.

European crystallographers are offered crystal dehydration at a number of synchrotron sources that are working together to further develop and enhance this method. The various implementations of the HC1 dehydration devices are presented as well as examples of the successful application of this method. By working together it is hoped that general protocols and automated routines can be further developed and presented to the user community through a common interface.

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[2] Sanchez-Weathersby et al. (2009), Acta Cryst. D 65, 1237-1246
[3] Russi et al.(2011), J. Struct. Biol.**175**, 236-243.
[4] Wheeler et al. (2012), Acta Cryst. F**68**, 111-114.

Keywords: macromolecular crystallography, synchrotron X-ray diffraction, dehydration