

Poster Presentations

[MS10-P20] Handling difficult samples: data processing improvements.

Fraser White,^a Daniel Baker,^a Zoltán Gál,^a Oliver Presly,^a and Mathias Meyer,^b

^a*Agilent Technologies UK Ltd, 10 Mead Road, Oxford Industrial Park, Yarnton, Oxfordshire, OX5 1QU, UK,*

^b*Agilent Technologies Sp. z o.o., Szarskiego 3, PL-54-610 Wrocław, Poland*

E-mail: fraser.white@agilent.com

A research project will often define at its inception a material or family of closely related materials for study. Sometimes obtaining crystal structure(s) is deemed to be highly useful and of high importance, yet unforeseen problems in obtaining high quality diffraction data can lead to difficulties in realising project goals. This may be for a number of reasons such as sample sensitivities, a propensity for twinning or simply weak diffraction.

It is therefore of great importance to have, not only a diffractometer capable of providing the best possible data from the sample, but also powerful software which can extract the maximum information possible from that data.

The CrysAlis^{Pro}[1] software package contains many tools and features for data processing which are designed to achieve these goals. The algorithms which underpin these tools are under continual development with new methods investigated and added to make getting the best quality data as easy as possible.

Some recent advances and results are presented herein.

[1] Agilent Technologies, CrysAlis^{Pro} Software system, **2013**, Agilent Technologies UK Ltd.