

# Poster Presentations

**[MS45-P12] Service Crystallography – Right tools for the challenge.** S.J. Coles, P.A. Gale, G.J. Tizzard, P.N. Horton, M.B. Pitak and S.J. Milsted,

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This poster will outline the capabilities of the UK National Crystallography Service (NCS, <http://www.ncs.ac.uk>)[1], based in Chemistry at the University of Southampton and one of only a very few funded, university-based national facilities which currently exist around the world. Single crystal diffraction is a valuable technique that underpins chemical science, which nowadays is used much more than to just determine a structure due to having a good crystal i.e. we have to work with what we are given! For example many functional materials only afford solid products that most would consider to be a powder (but often contain single crystallites) and in systematic studies it is vital to collect data on every member of a set. As such, the requirements of a service crystallographer have changed and recourse to more powerful facilities than the home laboratory is a common necessity. The NCS is fundamentally supported by state-of-the-art instrumentation (an entirely new facility was established in Sept 2011) that forms the most powerful laboratory-based chemical crystallography facility in the world. In collaboration with Rigaku, we have built an ultra high flux dual port molybdenum FR-E+ rotating anode equipped with bespoke focusing mirrors and the new High Gain Saturn 724+ CCD detector. This is complemented by a copper-based 007HF rotating anode (Saturn 944+ CCD detector) and a RAPIDII image plate system mounted on a sealed tube source. This equipment base also acts as a screen for a follow-on service for particularly testing samples at the Diamond Light Source (beamline I19). Access to I19 occurs regularly (about once a month) and is

totally seamless (no input required from sample providers) – around 17% of samples are examined in this way. Comparison tests have been carried out, that allow for a judgement between the capabilities of the various instrumentation and indicate approximately two orders of magnitude flux difference between I19 and the FR-E+. The NCS is one of the highest throughput facilities in the world, examining around 1200 samples a year (but with the total Southampton laboratory output being above 2000) and is supported by four dedicated research scientists, each of whom also pursue personal research programmes, and an administrator. Access to the NCS is based on peer reviewed proposals, with the primary services of either ‘Data Collection Only’ for those who wish to work up their own structures but are unable to collect suitable diffraction data on local facilities, or a ‘Full Structural Analysis’ where we work in collaboration to provide structural analysis all the way through to publication. We will attempt ANY sample and assure a rapid turnaround time, and welcome visitors, both to Southampton and Diamond, who wish to experience and learn the capabilities of the facility for themselves.

[1] Coles, S.J. & Gale, P.A., *Chem. Sci.*, 2012. DOI: 10.1039/C2SC00955B

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