

## Guidelines for users of the X-ray Crystallography Service

For any queries relating to the X-ray Crystallography service please contact Dr Claire Wilson, room B2-27b, Joseph Black Building [Claire.wilson.2@glasgow.ac.uk](mailto:Claire.wilson.2@glasgow.ac.uk) (extn 3214, external 0141 330 3214). The single crystal facilities are located in A4-19.

### **Sample submission procedure**

Please complete a sample submission form for each sample, available [here](#) or from Claire Wilson, giving as much information as possible including possible contaminants, starting materials or alternative products, with unit cell parameters if known.

### **Suitable samples**

Lots of tips and advice are available online on growing crystals – for example ‘*Growing Crystals that will make your crystallographer happy*’ by Paul Boyle <http://crystallography.usc.edu/growingcrystals.pdf> and others by Sandy Blake <http://www.nottingham.ac.uk/~pczajb2/growcrys.htm> and by Martin Lutz <http://www.cryst.chem.uu.nl/lutz/growing/growing.html>.

If you would like to check whether your crystals are suitable for analysis please contact Claire. ‘Suitable’ or ‘good’ crystals generally means single crystals around 0.2 - 0.5mm in size; larger crystals can be cut and smaller crystals may also be possible to analyse, depending on the material or through the National Crystallographic Service allocation. If possible, keep some of the mother liquor with the crystals – in many cases solvent molecules are incorporated into the lattice and if the crystals dry out the quality may deteriorate.

Better crystals generally means better quality results which are more likely to allow the information required to be determined and make publication more straightforward. Crystals that grow more slowly – slower cooling, evaporation, from more dilute solutions – often give fewer but better and larger crystals so take your time.

Submit samples in a container that the crystals can be removed from straightforwardly – please avoid large round bottom flasks, vials that are too narrow for a spatula – especially screw top ones, excessive quantities of solvent.

Other characterisation data – NMR, MS, IR, elemental analysis – should be obtained to determine the chemical composition and will be required for publication of new compounds. Techniques such as NMR and/or powder diffraction should be used to establish whether the material is pure and whether single crystal is representative of the bulk material.