

**Service Level Agreement for the Small Molecule X-ray  
Crystallography Service  
School of Biological and Chemical Sciences  
Queen Mary University of London**

**Contact**

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**Definition of Service**

The Small Molecule X-ray Crystallography Service provides crystal structures of small molecules in a timely and effective way. Use of the service is taken as recognition of the fact that the accuracy of the crystal structure (the resolution and the extent to which the refined crystal structure accounts for the measured intensities) ultimately depends on the quality of the crystals provided by the user and the inherent order in the small molecule and the surrounding water and other solvent and salt molecules.

**Service provided**

We shall produce a crystal structure of the small molecule and provide coordinates, a cif check report, and a picture of the compound. For many small molecules lacking molecular and solvent disorder we shall provide a fully refined structure suitable for publication in a refereed journal. However, this will not always be possible. At this stage the user will be told if the structure is of suitable quality for publication in a journal requiring crystallographic data to be refereed.

**User responsibilities**

It is the user's responsibility to provide crystals suitable for crystallographic structure determination. The user should also provide details of the anticipated chemical formula of the molecule and the nature of the solvent. Please note that when it is suggested effort is put into obtaining better crystals, the quality of the resulting structure will also be substantially better. The user is responsible for furnishing details of hazards associated with the submitted compound in line with COSHH regulations.

**Confidentiality**

Communications concerning the identity of the small molecule and its structure will be kept confidential and not revealed to any third party. We shall sign appropriate confidentiality agreements with commercial users

**Publication and Acknowledgements**

Where the service provider has made a contribution to the work, one that is worthy of authorship, the service provider will be a co-author on resultant publications. In all other cases the service should be acknowledged as follows: "We acknowledge use of Queen Mary University of London, School of Biological and Chemical Sciences Small Molecule Crystallography Service."

**Problem management**

The user can approach Dr I Abrahams or Prof RW Pickersgill in the case of any concern, for conflict resolution, or for disaster recovery.