A Novel Method to prepare Iodine Derivatives for In-house Phasing

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We developed novel procedures for efficient preparation of iodine derivatives of protein crystals that are most effectively employed for in-house phase determination. In this procedure, target native crystals are exposed by gaseous iodine. In the crystals, hypoiodous acids are generated, and they form covalent bonds at the *ortho*-positions of accessible tyrosine residues by the aromatic electrophilic substitution. The resultant iodine derivatives are the most suitable for in-house phasing using longer wavelength X-rays, such as Cr-Ka X-rays, because anomalous signals of iodine are strengthen at the region of longer wavelength X-rays.

We applied this approach to native crystals of thaumatin. The crystals were successfully iodinated to generate enough phasing power by the Cr-Ka X-rays. As a result, the crystal structure of the iodinated thaumatin was solved by fully automated procedure. The present methods not only to contribute to the in-house *ab initio* structure determinations using Cr-Ka radiation, but also to promote the phasing at synchrotron facilities if their beamlines provide longer wavelengths than the conventional ones. In the poster session, the possibility of the present method to apply for other crystals will be discussed.

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