Pharmaceutical Application of Synchrotron X-ray Powder Diffraction at SPring-8

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We have performed the *ab-initio* crystal structure determination of phamaceutical compounds from powder data collected by an Imaging Plate system of large Debye-Scherrer camera at BL19B2. Use of synchrotron radiation has the important advantage of using variable wavelength for data collection with a highly pararell beam.

As a standard sample, cimetidine ($C_{10}H_{16}N_6S$) and trehalose dihydrate (C_{12} H_{22} O_{11} $2H_2O$) are used, and their crystal structures are significant-

ly solved by the method of Simulated Annealing (*DASH* and *Powder Solve*) and also by the direct method (*EXPO2004*). After Rietveld refinement, refinement parameters of trehalose dehydrate data is *Rp*=2.27, *Rwp* = 3.4 [1]

Using Imaging Plate system rapid data collection of 2- 5 minute exposure is sufficient for structure determination and continuous data collection at different temperature is easily occupied.

We have also been planning to determine in-situ structure determination in transition of trehalose dehydrate at high temperature and under humidity control [2].

These results suggest that the powder diffraction system at BL19B2 is useful for pharmaceutical solids including polymorph and its phase transition.

[1] Altomare A., et al., *J Appl. Cryst.*, 2004, **37**, 1025-1028. **[2]** Kishi A., Toraya H., *The Rigaku Journal*, 2004, **21**, 25-30.

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