

SS02-4 **Structure determination of pharmaceutical compounds from powder diffraction data using SPring-8**

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Polymorphism in pharmaceutical compounds is very important, because there have been serious problems of stability and physicochemical property in process analytical technology.

Recently, many successful results of crystal structure determination in polymorph from powder diffraction data are reported. It depends the progress of data collection and software for analysis. We are now able to simulate crystal form by bulk powder without large-sized single crystal.

We have been collecting high resolution powder diffraction data at BL19B2/SPring-8 in industrial application proposals since 2005, and succeeded in crystal structure analysis of Tolbutamide¹⁾ and Acrinol²⁾ with phase transition.

With dihydrated Lisinopril, according to its results of XRD-DSC, we have collected sequential temperature dependent powder diffraction data at BL19B2 and determined its dehydration steps with crystal structures and water channel. We hope our results enhance many researches with powder diffraction in pharmaceutical field.

1) G. Hasegawa, T. Komasa, R. Bando, Y. Yoshihashi, E. Yonemochi, K. Fujii, H. Uekusa and K. Terada, *Int. J. Pharm.*, 369, 12-18(2009).

2) K. Fujii, H. Uekusa, N. Itoda, G. Hasegawa, E. Yonemochi, K. Terada, Z. Pan and K. D. M. Harris *J. Phys. Chem. C*, accepted