

STRUCTURE SOLUTION AND QUANTITATIVE X-RAY POWDER DIFFRACTION OF PHARMACEUTICALS

Dr Gregory Stephenson, Eli Lilly & Company

A metastable form of research compound was discovered. Due to the nature of isolation, crystals of sufficient size for single crystal diffraction could not be grown. The X-ray powder diffraction pattern was indexed using X-cell and was subsequently solved using the Powder solve. Futhermore, a variety of quantitative methods were applied to assess the relative merits of approaches such as Rietveld analysis, whole pattern least squares refinement, chemometric and single peak methods.