

A Novel Approach of Using Powder X-ray Diffraction for High-Throughput Crystallization/Salt Screening

Shawn Yin¹, Vic Rosso¹, Anne Song¹, Jack Venit¹ and Holger Cordes²

1- Bristol-Myers Squibb Company, 2- Bruker-AXS Inc.

Abstract

Characterizing the hits obtained from high throughput crystallization/salt screening by powder X-ray diffraction (PXRD) has generated significant interests from pharmaceutical industry. The traditional 96 well plates for high throughput crystallization limited the applications of physical characterization tools to this area. This presentation will describe a novel, patent pending design of 96 well plate used on a transmission model powder X-ray diffraction instrument with area detector, for high throughput crystallization/salt screening process. The glass bottom 96 well plate allows the chemical reaction, crystallization and all non destructive physical characterizations being accomplished inside the same cell without transferring samples from one place to another. This approach has the capability of generating PXRD patterns with the comparable quality to other sample/instrument configurations, for sample size as low as 0.25 mg. And the mixed polymorphic forms can also be distinguished.