

Rapid XRD Screening for Combinatorial Chemistry on the Millisecond Time Scale

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The combinatorial chemistry approach to new product development has increased dramatically over the past several years. Using this technique it is possible to explore thousands of samples in a much shorter time period compared to conventional synthetic routes. Due to the large array of samples that are produced, the combinatorial chemistry approach requires rapid screening techniques to test and evaluate the variation of composition, structure and properties across the combinatorial library.

At present, a state of the art XRD system with a 2-dimensional general area detector diffraction system (GADDS) can perform accurate phase identification on diffraction data collected as fast as 30 milliseconds. Additionally, with the use of pinhole collimators, this system can analyze small samples with an incident beam diameter as small as 10 microns.

In this publication the threshold of speed and accuracy in the analysis of combinatorial chemistry libraries have been explored by XRD. Time resolved studies varying data collection times from 30 milliseconds up to several minutes are compared with respect to the structural information they provide for several sample types. In addition, time resolved quantification using a standardless method has been explored on several sample types.