Total Pattern Analyses of Pharmaceutical Formulations

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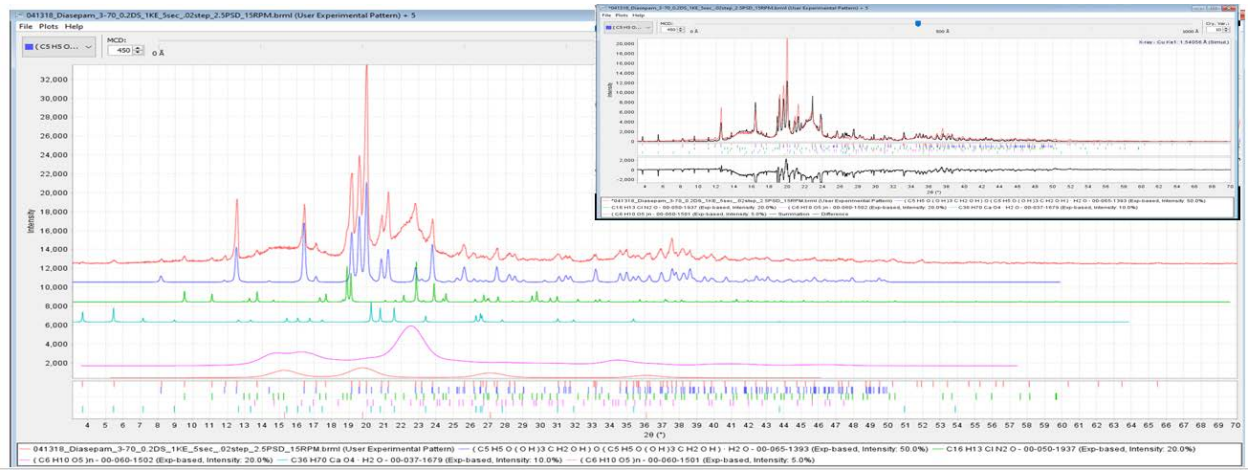
Diffraction analyses of pharmaceutical formulations have historically been hindered because of the wide spread use of non-crystalline and nanocrystalline ingredients and the difficulties in analyzing these materials. To address this issue the International Centre for Diffraction Data, over the last decade, has developed a system for analyzing whole patterns containing noncrystalline materials. The system includes several components; 1) the systematic additional of experimental pattern references for noncrystalline API's and excipients, 2) the development of application software that can correct for common instrumentation and specimen effects 3) a suite of graphics programs to scale, sum and display various combinations of reference and experimental data. Reference pattern simulations include adjustments for crystallite size and orientation.

To evaluate the effectiveness of the analysis applications, 65 pharmaceutical formulations were analyzed. The poster will demonstrate total pattern analysis for several of these formulations including those containing the most commonly occurring excipients. The analyses were conducted on high volume pharmaceutical including Azor®, Prilosec® OTC, Tramadol®, Eliquis®, Singulair®, Diazepam®, Invokana®, Myrebetriq® and Seroquel®.



The X-ray powder diffraction pattern of Diazepam® (top red pattern) compared to the reference patterns of its identified ingredients, lactose monohydrate, diazepam, calcium stearate, cellulose 1β, amorphous cellulose. The insert shows a comparison of summed phases (black) to the experimental data (red).