

PHARM007: Polymorph Quantification by the DD Method without a Calibration Curve

Introduction

In drug development and quality evaluation, quantifying trace components and polymorphs is essential. However, preparing calibration curves and obtaining crystal structure information can be a significant burden. The Direct Derivation (DD) method is effective in addressing these issues. It can quantify the components of a mixture using only X-ray diffraction data and chemical formulas of pure substances, eliminating the need for calibration curves and structural information.

Crystalline phase analysis

Analysis:	Active pharmaceutical ingredients
Use:	Pre-formulation (API)
Analyzed materials:	Carbamazepine (CBZ)
Analysis software:	SmartLab Studio II

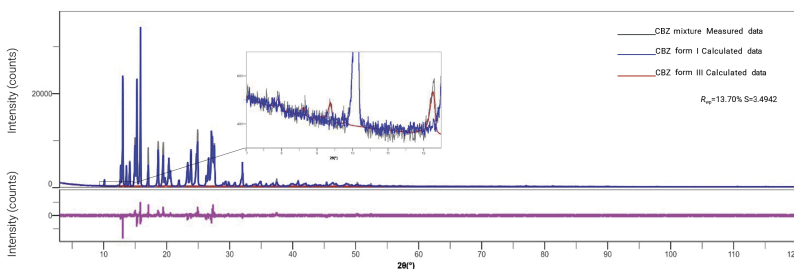


Figure 1: Refinement calculation results for CBZ mixture (prepared values: Form I 99.00 wt%, Form III 1.00 wt%)

Conclusion

Figure 1 shows a profile with carbamazepine Form I with 1.00 wt% Form III. By applying the DD method to this measurement data, a highly accurate quantitative result of 0.99 ± 0.09 wt% was obtained. The DD method enables simple and high accuracy quantification using only XRD data and chemical formulas of pure substances, without the use of calibration curves or structural information. This makes it effective for the evaluation of impurities produced in the synthesis process.

Related products



SmartLab

Advanced state-of-the-art high-resolution XRD system powered by Guidance expert system software



SmartLab Studio II

Windows-based software suite for Rigaku's X-ray diffractometers