



**Malvern  
Panalytical**  
a spectris company

# Aeris in Pharma

Solid-state characterization of small molecule pharmaceuticals



# Solid-state characterization of small molecule pharmaceuticals

Regulated environment solution: OmniTrust

Aeris Compact XRD

Analytical method development: HighScore

## Aeris Compact XRD

### Modern solid-state analysis

In small molecule drug development, speed-to-market is crucial. With tightening regulations, efficiency and safety are paramount. At Malvern Panalytical, we listen to our customers to bring you solutions tailored to your needs. Through collaboration between X-ray diffraction and pharmaceutical industry experts, we've developed a total XRD solution that will give your team confidence no matter what the analytical or regulatory challenges you are facing.

The main advantage of having an Aeris available to us is the fast turnaround of samples. The machine has become a true workhorse in our lab to follow up crystallization outcomes at different stages of the process, and in different phases of development. Having the Aeris available to us we can do routine phase identification measurements in an accessible and operator friendly manner."

Aeris user working in process development for API manufacturing



### Maximum efficiency with speed and accuracy

Aeris combines easy external sample handling with clear, simple, push-button operation. Featuring an integrated computer and a classic goniometer, Aeris delivers high-performance scans and robust, repeatable data in minutes.

### Simplify your workflow

With Aeris, you can introduce samples manually or via fully integrated automated systems. Sample holders are easily and precisely handled via external positioning stations and can be changed without interrupting ongoing measurements. With multilevel user accounts, preprogrammed measurement methods, and an easy-to-use touchscreen, you don't need to be an XRD expert to generate repeatable, reliable results from Aeris.





## Higher-quality powder data

### Standard method: Reflection

Combining low noise, high resolution, and true reproducibility, Bragg-Brentano measurements reveal new insights into your materials' structure-property relationships. This data can take you all the way from phase identification to crystal structure solution.

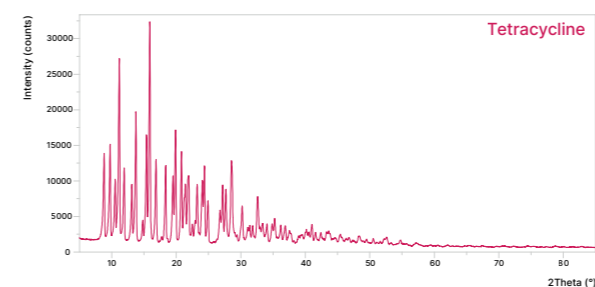


Figure 1. Bragg-Brentano measurement (reflection mode) of tetracycline hydrochloride.

### Challenging samples: Transmission

Transmission measurements allow you to minimize preferred orientation effects. Also, this geometry is particularly beneficial for low-absorbing organic materials, as it prevents challenges with sample transparency.

Reflection pattern in Figure 2 is indicating strong preferred orientation and is lacking majority of reflections, whereas transmission measurement is highly comparable with a theoretic pattern.

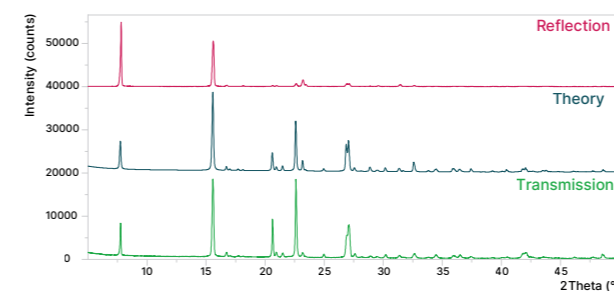


Figure 2. 2-Acetoxybenzoic acid (aspirin) measured in reflection and transmission mode and a calculated pattern for comparison.

### Unchallenged sensitivity: Detection limits

When working with drug substances or products, detecting potential polymorph contamination is crucial. Aeris' high sensitivity ensures you can identify these issues, enhancing product quality and minimizing risks. With its low background and high resolution, Aeris allows you to routinely screen your materials for low-level impurities. Figure 3 shows two XRD patterns of indometacin / lactose formulation, measured in reflection mode. In the zoomed in fragment one can clearly see additional reflection, corresponding to a different, not efficacious polymorph of indometacin -  $\alpha$  form - as opposed to efficacious  $\gamma$  form.

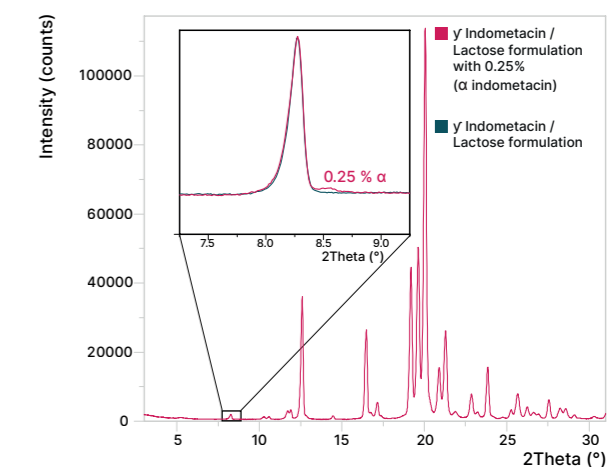
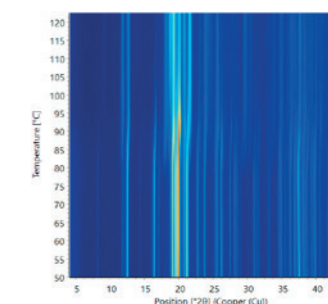


Figure 3. XRPD patterns of indometacin / lactose formulations.

### Stability assessment at variable temperature

Stability evaluation of drug substances and products is a critical step in developing small molecule pharmaceuticals. These studies predict the phase behavior of both drug substance and formulations, helping to anticipate their shelf life.

Early stability assessments through *in situ* non-ambient experiments allow you to focus on the most promising candidates, saving time and effort by discarding meta-stable substances long before extensive stability evaluations of marketed or ready-to-release pharmaceuticals are conducted.



# OmniTrust

## 21 CFR Part 11 compliance built in

We understand the importance of data integrity in regulated environments, from instrument qualification to compliance and auditing. Our OmniTrust solution supports multiple analytical instruments, including Aeris, ensuring record accuracy and best practices in data integrity.



**OmniAccess**  
System configuration &  
role management



**OmniTrail**  
Viewing system  
audit trails



### Instrument & Analytical software

**XRDMP Creator** Creation of measurement programs  
**Aeris Instrument Suite** Running measurements

**Data Viewer** View & review of measurements  
**HighScore** Data analysis

## Ensuring data integrity

Designed with industry experts, OmniTrust defines user roles according to your workflow and tracks every interaction with Aeris, from creating measurement routines to reviewing data. System controls prevent errors and ensure regulatory compliance. Potential issues with data integrity are instantly identifiable and accessible for review, saving you time and reducing stress.

## Central Management with OmniTrust

Subscribe to OmniTrust's Central Management feature to analyze both analytical and audit trail data from multiple instruments anywhere. By bringing multiple analytical instruments into the same environment, you benefit from:

- Central setup of instruments and workstations
- Unified roles and permissions across the lab
- Comprehensive audit trails from all systems

## NEW: Mastersizer and Revontium join OmniTrust family!

Expand your OmniTrust universe beyond Aeris! OmniTrust is now also available on laser diffraction instrument Mastersizer and energy-dispersive X-ray fluorescence spectrometer Revontium. No more struggling with different regulated environment solutions—enter the OmniTrust world and enjoy a unified system and user configuration platform.



# Analytical method development

## HighScore: For every analytical challenge

HighScore Suite is an analytical software package designed for users of all experience levels in X-ray powder diffraction. It allows you to handle a wide range of analytical tasks, including

- Phase identification
- Phase quantification (from single to multiple crystalline and/or amorphous phases)
- Testing for limits of detection
- Crystallinity determination
- Structure solution
- Cluster analysis

From pattern overlay to structure solution, in fully or semi-automated mode or completely manually – the choice is yours!

Our team of application scientists can help you develop analytical methods tailored to your specific needs.



Get in touch with our experts now!



## About Malvern Panalytical

Malvern Panalytical is a global leader in the analytics of material and life sciences. We unleash the power of small things to make big things happen for our customers.

Our vision is to make the world cleaner, healthier, and more productive.

We partner with our customers to make their solutions possible through the power of precision measurements, our expertise, trusted data, and insights.

Our people are partners in discovery. We collaborate with our customers and with each other to discover new possibilities and achieve breakthroughs.

Our culture is a healthy, high-performance culture shaped by our values: Own it, Aim High and Be True.

We're committed to Net Zero in our own operations by 2030 and in our total value chain by 2040.

With over 2300 employees across the globe, we are part of Spectris plc, the world-leading precision measurement group.

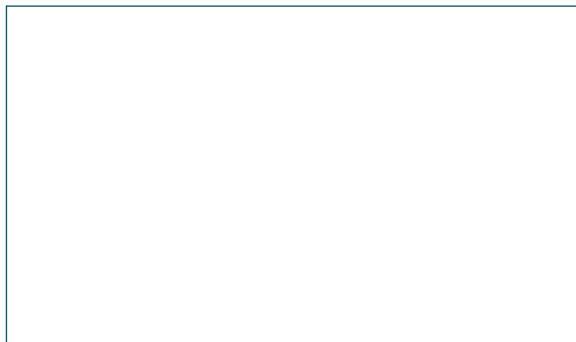
**Malvern Panalytical. We're big on small™**

## Service & Support

Malvern Panalytical provides the global training, service and support you need to continuously drive your analytical processes at the highest level. We help you increase the return on your investment, and ensure that as your analytical requirements grow, we're there to support you.

Our worldwide team of specialists adds value to your business processes by ensuring applications expertise, rapid response, and maximum instrument uptime.

- Proactive local and remote support
- Full and flexible range of service agreements
- Compliance and validation support
- Onsite or classroom-based training courses
- e-Learning training courses and web seminars
- Digital services, including MyStore and My Customer Support Portal
- Sample analysis, method development, and applications consultancy



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