

# Ensuring safer and effective pharmaceutical formulations by X-ray diffraction

From drug discovery and preformulation studies to the efficient scaling up in the manufacturing process in the plant and finally through QA/QC validation, X-ray diffraction (XRD) is a vital analysis method in the characterization of different physico-chemical properties of the active pharmaceutical ingredient (API).

XRD is a gold standard method and required technique in the determination of polymorphic and salt screening, % of crystallinity and stability/reactivity studies of the final API. XRD is also utilized in pharmaceutical forensics to identify and detect counterfeit drugs and additives. Since X-ray diffraction provides a characteristic fingerprint of crystalline phases and their relative concentrations, it is a powerful tool not only for R&D laboratories but also the downstream processes providing the same methodology, libraries and data integrity at all steps in the pipeline.

In particular, in-situ or real-time XRD is useful in studying the reactivity/stability of API formulations along with structural phase transitions occurring in the material under a controlled environment. Given the nature of organic materials, it is also extremely useful to perform transmission X-ray diffraction (on tiny samples or small quantities available for analysis).



In summary, XRD is a powerful technique to structurally characterize a pharmaceutical compound throughout the drug product pipeline.

**!** **NOW AVAILABLE • 21 CFR Part 11 compliance**  
 The new Thermo Scientific™ SolstiX™ XRD Software with Security Suite for Thermo Scientific™ ARL™ EQUINOX X-ray Diffractometers enables compliance with FDA 21 CFR Part 11 regulations to confidently secure your laboratory data and its integrity: [thermofisher.com/solstix](http://thermofisher.com/solstix)

## Top applications for pharma

- Crystallography and crystal structure determination
- Phase analysis and polymorph screening
- Crystallinity determination
- Solid dosage forms and bioavailability
- Stabilities studies
- Manufacturing and production
- Process control

## Top XRD benefits for pharma

- Structural characterization technique
- Nondestructive technique
- Small amount of sample needed for analysis
- Unique diffraction patterns and quick response
- Analysis on mixtures as well as amorphous content
- Easy determination of induced structural changes

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## Thermo Scientific™ SolstiX™ XRD Software with Security Suite extends ARL EQUINOX X-ray Diffractometers to 21 CFR Part 11 regulated labs

- Protect stored **electronic data** related to quality assurance within manufacturer's computer systems
- Put controls in place to keep records authentic, incorruptible, and confidential
- **Electronic signatures** for the user to take responsibility for the electronic data in the system
- Requirements in the data record: date and time of scan, name of the unique signer, and technological controls to ensure security (e.g. passwords)

## Thermo Scientific™ ARL™ EQUINOX X-ray diffractometers are designed to exceed your analytical needs

- Ideally suited for rapid screening of various formulations, finger printing or detection of counterfeit products
- Polymorphism and crystallinity determination, crystallite size calculation, quantitative phase analysis, reactivity and stability of materials, etc.



### Thermo Scientific™ ARL™ EQUINOX 100 XRD for structural analysis

- Easy-to-use simultaneous full pattern XRD based on unique real time PSD detector technology
- Unique dual-mode capability on a benchtop XRD instrument: reflection and/or transmission mode
- XRD experiments on standard powders, tablets, small quantities, with sample spinner, capillary stage, sample changer or in controlled environment

### Thermo Scientific™ ARL™ EQUINOX 1000 XRD for increased sensitivity

- Real-time full pattern acquisition of a pharmaceutical sample in few seconds to minutes
- Reflection or transmission mode with monochromator optics for higher resolution or intensity
- Various sample stages for dynamic studies of powders or tablets in controlled environment
- 30-position sample changer for routine or batch operation



### Thermo Scientific™ ARL™ EQUINOX 3000 XRD for R&D laboratory

- Floor-standing standard powder XRD for real-time detection with higher resolution
- Full flexibility to measure pharmaceutical samples under controlled environment, humidity or with low/high temperature chambers
- Transmission or reflection XRD with flexible monochromator or mirror optics for optimum resolution/intensity
- In-situ measurements with fast acquisition of full XRD pattern for reactivity and stability tests

Find out more on XRD solutions at [thermofisher.com/xrd](https://thermofisher.com/xrd)  
and our broader portfolio at [thermofisher.com/pharma](https://thermofisher.com/pharma)

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