

## X-ray diffraction

## 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.

### 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

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 ready

The new Thermo Scientific™ SolstiX™ XRD Software with Security Suite for Thermo Scientific™ ARL™ EQUINOX 100 X-ray benchtop Diffractometer enables compliance with FDA 21 CFR Part 11 regulations to confidently secure your laboratory data and its integrity: [thermofisher.com/solstix](https://thermofisher.com/solstix)

### 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



## Thermo Scientific™ SolstiX™ XRD Software with Security Suite extends ARL EQUINOX 100 X-ray Diffractometers to 21 CFR Part 11 regulated labs

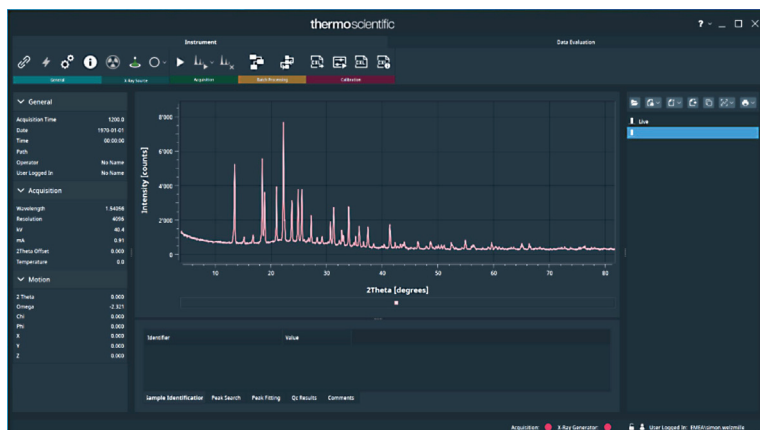
- Protect stored electronic data related to quality assurance within manufacturer's computer systems
- Put controls in place to keep records authentic, incorruptible, and confidential
- Electronic signatures for the user to take responsibility for the electronic data in the system
- Requirements in the 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 100 X-ray benchtop diffractometer is 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.
- XRD experiments on standard powders, bulks, tablets, small quantities, etc.
- Real-time full pattern XRD based on our unique PSD detector technology
- X-ray source based on micro-source technology with no external water cooling
- Unique dual-mode capability: reflection and/or transmission

## 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 various samples with sample spinner, capillary stage, sample changer or in controlled environment



SolstiX software control screen, Taurine sample.

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)