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.

Top 5 XRD applications for pharma
- Discovery
- Quality control
- Crystallinity
- Solid dosage forms
- Bioavailability

Top 5 XRD benefits for pharma
- A structural characterization technique
- Non destructive
- Unique diffraction patterns
- Can analyze mixtures as well as amorphous content
- Easy determination of induced structural changes
Thermo Scientific XRD solutions for structural analysis of pharmaceuticals

**Thermo Scientific™ ARL™ EQUINOX 1000 X-Ray Diffractometer 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
- Requires external water chiller

**Thermo Scientific™ ARL™ EQUINOX 1000 X-Ray Diffractometer for structural analysis**
- Easy-to-use simultaneous full pattern XRD based on unique detector technology without motorization
- Unique dual-mode XRD capability on a benchtop instrument: reflection or transmission XRD
- Can perform XRD experiments on standard powders, tablets, small quantities, with capillary stage or in controlled environment
- Ideally suited for rapid screening of various formulations, fingerprinting or detection of counterfeit products
- Can be used to determine polymorphism, crystallinity, crystal size, quantitative phase analysis, reactivity and stability of materials

**Thermo Scientific™ ARL™ EQUINOX 3000 X-Ray Diffractometer for R&D labs**
- 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
- Requires external water chiller

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