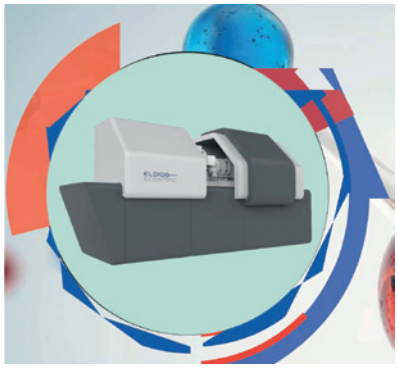
Electron Diffraction
Structure determination directly from nanocrystalline powders



Electron diffraction (3D ED, microED) is the most recent addition to the crystallographic toolkit and allows researchers to determine crystal structures directly from nanocrystals of sizes around 50-1000 nm. The world's first dedicated electron diffractometer, the ELDICO *ED-1*, makes this technology easily accessible to everybody and has already helped scientists across many fields in their research endeavours.

The future of electron crystallography

Single crystal X-ray diffraction (SC-XRD) is the standard technology for structural characterisation in the solid state, but requires single crystals of suitable size (typically at least 10 µm in the smallest dimension on laboratory sources). In contrast, the stronger interaction of electrons with matter allows 3D ED to perform structure elucidation on samples with crystallite sizes far below 1 µm, which is out of reach even for the largest synchrotron facilities. This means that powder samples can be analysed straight "from the flask" without the additional step of growing large crystals – which can be very resource- and time-consuming and sometimes even impossible as many experimentalists will have experienced. Despite this potential, 3D ED has long been a topic for specialists due to the difficulty of performing such experiments on existing transmission electron microscopes (TEMs). The ELDICO *ED-1*, the world's first dedicated electron diffractometer, unlocks the full potential of electron diffraction and makes the technology available to crystallographers around the world without the need of being an electron microscopy expert.

The unique horizontal design of the ELDICO *ED-1* is optimised for diffraction experiments. The highly precise goniometer can centre any point of interest on a TEM grid or alternative sample support in the electron beam, while an ultrafast and noise-free detector (Dectris QUADRO) enables data collection in continuous rotation mode. STEM (scanning transmission electron microscopy) imaging mode ensures that the sample is exposed to the lowest possible radiation dose during searching and centering crystals. The lean electron optical system lets the user switch fast and easily between different beam modes. At the same time the setup is designed without any optics between sample and detector to avoid distortions in the diffraction pattern, which are common on TEMs. With these features, the ELDICO *ED-1* can produce superior data for 3D ED analysis and other electron crystallographic applications.

Selected publications with ELDICO *ED-1* data:

P. Sieger et al. *Eur. J. Pharm. Sci.* **2023**, *186*, 106447. https://doi.org/10.1016/j.ejps.2023.106447.

I. D. Williams et al. *Symmetry* **2023**, *15*, 983. https://doi.org/10.3390/sym15050983.

M. Gemmi et al. *Acta Cryst. B* **2023**, *79*, 432. https://doi.org/10.1107/S2052520623007680.

M. Rickhaus et al. *Nat. Commun.* **2023**, *14*, 4725. https://doi.org/10.1038/s41467-023-40475-8.

M. Pop et al. *CrystEngComm* **2024**, *26*, 4295–4304. https://doi.org/10.1039/D4CE00518J.

B. A. Palmer et al. *Cryst. Growth Des.* **2024**, *24*, 899. https://doi.org/10.1021/acs.cgd.3c01290.

B. Thomas et al. *Chem. Sci.* **2024**, *15*, 16015–16024. https://doi.org/10.1039/D4SC05453A.

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ELDICO SCIENTIFIC

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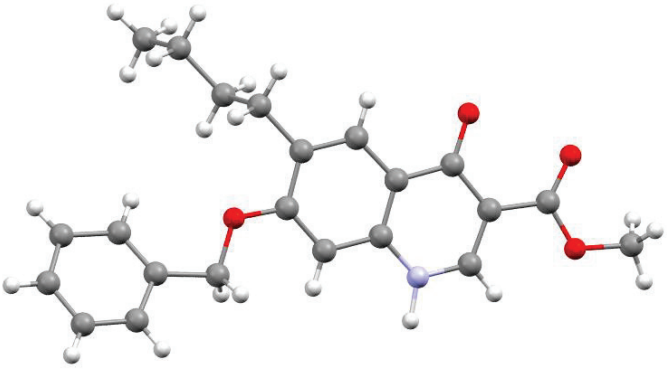
Case Study: Nequinate

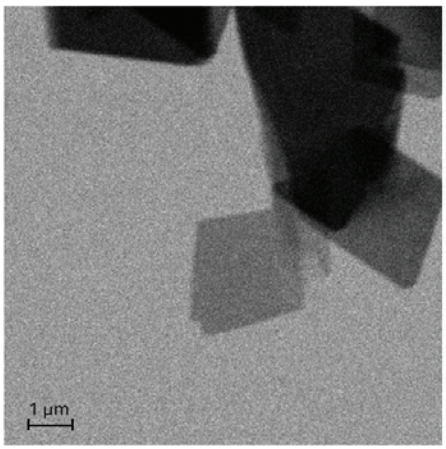
Electron diffraction made easy

With the ELDICO *ED-1* crystal structures can be obtained from any crystalline powder material, as shown here for nequinate – an antiprotozoal drug. A powder sample from a commercial supplier was prepared as is on a standard TEM grid (amorphous carbon on copper) and measured on an ELDICO *ED-1* electron diffractometer. Data were processed (Bruker Apex4, SAINT and SADABS), solved (ShelXT), and refined (SheXL) with standard crystallographic software and are compatible with all major software packages. Nequinate crystallises in monoclinic space group $P2_1/c$ with unit cell parameters of a=18.3(2), b=11.71(13), c=9.07(10), and β=99.324(18). The process from sample preparation to structure took less than 60 minutes.

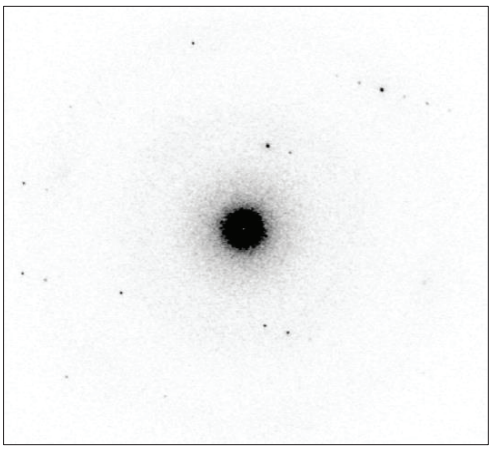


Molecular structure of nequinate from ED data

Nequinate powder sample

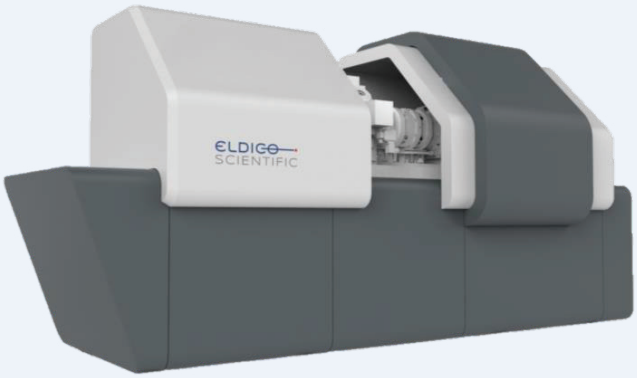


STEM image of nequinate crystallites



Diffraction frame from a nequinate crystallite

The ELDICO *ED-1* – designed by crystallographers for crystallographers



- ✓ **easy to use**
- ✓ **unique horizontal design**
- ✓ **highly precise goniometer**
- ✓ **low-dose STEM imaging**
- ✓ **noise-free detector**
- ✓ **superior data quality**
- ✓ **flexible for customisation**

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