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Circular Dichroism beamline provides breakthrough in mapping chiral materials

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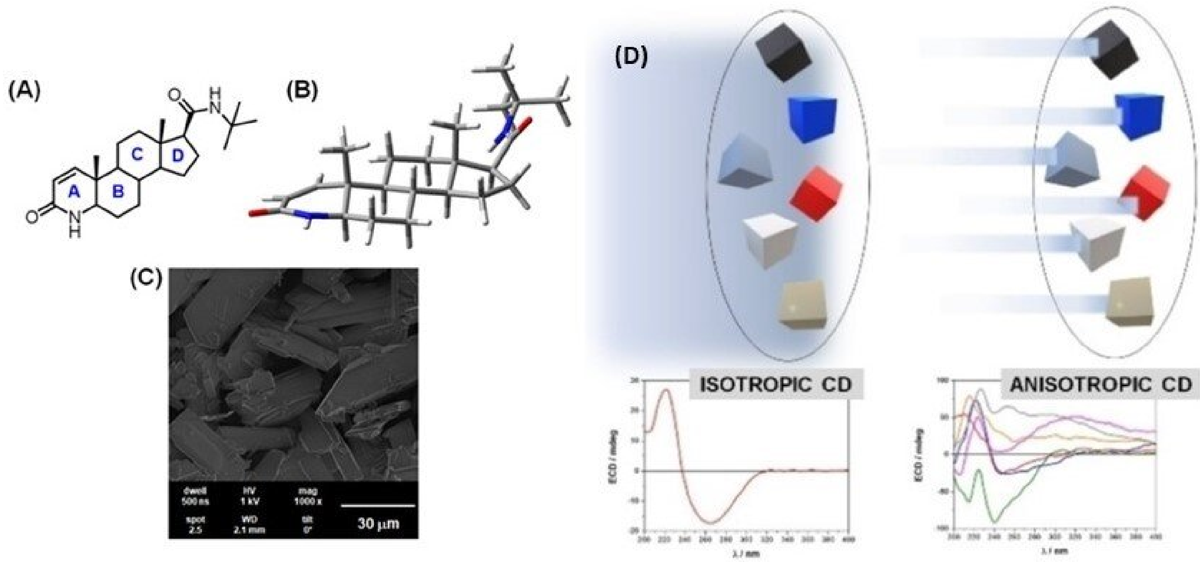

2D structure (A), 3D X-ray structure (B), and scanning electron micrographs of the crystal form I of finasteride (C), and CD spectra of the sample in solution (isotropic) and in the microcrystalline form (anisotropic), of which the latter can only be measure with B23 beamline unattainable with bench-top CD instruments (D). Credit: DOI: 10.1002/chem.202103632

A European research group has developed an exciting new imaging method on Diamond Light Source's beamline B23 that could improve the characterisation of chiral molecules in pharmaceuticals and other chiral molecules in the solid state. This pioneering work may have important impact on drug development and control of illegal substances by allowing the identification of a specific 'fingerprint' for each molecule.

Development of this important new tool was only made possible by the combination of Electronic Circular Dichroism (ECD) imaging together with the highly collimated microbeam generated at the Diamond B23 beamline which allowed higher spatial resolutions that were previously unattainable with earlier bench top instruments.

Optimizing the Circular Dichroism Imaging tool

Beamline B23 for Circular Dichroism at Diamond is a life sciences, chemistry and material science beamline for investigating and observing structural, functional and dynamic interactions in elements such as proteins, nucleic acids, nanoparticles and chiral molecules.

Circular Dichroism (CD) is an absorption spectroscopy technique that uses the differential absorption of left- and right-handed circularly polarized light to investigate the structure of chiral molecules. Electronic Circular Dichroism Imaging (ECDi) is one of the key techniques available to determine the configuration of small molecules, particularly chiral active pharmaceutical ingredients (APIs), and is now a vital tool in chemistry, physics and materials science providing unique information on chiral structures consisting of many molecules (supramolecular). Combining conventional CD instruments with synchrotron technology reduces the measurement time and amounts of sample material required for true chirality measurement and accurate identification of configuration. The new method should also be able to extract additional information from microcrystalline samples without the need for orientation of samples and single large crystals.

Harnessing the power of the synchrotron

In the new work, recently published in Chemistry—A European Journal, the team developed ECDi on the B23 beamline which enables the mapping of large sample surfaces at various spectral resolutions down to 0.01 mm^2 because of the highly collimated micro light beam available on the beamline. Previously, measuring the ECD of solid samples with bench top ECD instruments meant that the structural information of small domains (

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