

The CryoEM Method MicroED as a Powerful Tool for Small Molecule Structure Determination

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SUMMARY

UCLA researchers in the Department of Chemistry and Biochemistry have developed a novel use of the cryogenic electron microscopy (CryoEM) method electron micro-diffraction (MicroED) to provide routine and unambiguous structural determination of small organic molecules.

BACKGROUND

Nuclear magnetic resonance (NMR) spectroscopy has been a mainstay in chemistry and the most predominant method employed in both routine synthetic chemistry experiments and in advanced structural elucidation of complex small molecules. Single crystal X-ray diffraction produces unequivocal structural information about the position, orientation, connectivity, and placement of individual atoms and bonds within a given molecule. However, the use of X-ray diffraction is largely limited by the difficulty to produce high quality crystals amenable for X-ray diffraction. For this reason, X-ray diffraction has not been routinely used by most practicing organic chemists, despite that the structural data provided is superior to any other methods.

INNOVATION

Researchers at UCLA have developed a cryogenic electron microscopy (CryoEM)-based electron micro-diffraction (MicroED) method to address the need for fast and reliable structure determination in organic chemistry. They have demonstrated that with minimal sample preparation and experiment time, simple powders and amorphous materials could be directly used in MicroED studies, rapidly leading to high quality molecular structures at atomic resolution (<1 Angstrom).

APPLICATIONS

- Small molecule structure determination at atomic resolution

ADVANTAGES

- Faster and simpler preparation to acquire crystals
- High quality atomic resolution structures of complex, small molecules

STATE OF DEVELOPMENT

The described method has been experimentally validated.

PATENT STATUS

Country	Type	Number	Dated	Case
United States Of America	Published Application	2023-005790	02/23/2023	2019-360

RELATED MATERIALS

- Jones, C.G., Martynowycz, M.W., Hattne, J., Fulton, T.J., Stoltz, B.M., Rodriguez, J.A., Nelson, H.M. and Gonen, T., 2018. The cryoEM method MicroED as a powerful tool for small molecule structure determination. ACS central science, 4(11), pp.1587-1592.

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OTHER INFORMATION

KEYWORDS

Cryogenic electron microscopy,
 CryoEM, electron micro-diffraction,
 MicroED, structure determination,
 small molecule

CATEGORIZED AS

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