Small Molecule Microcrystal Electron Diffraction (MicroED) for the Pharmaceutical Industry – Lessons Learned from Examining Over Fifty Samples

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The emerging field of microcrystal electron diffraction (MicroED) is of great interest to industrial researchers working in the drug discovery and drug development space. The promise of being able to routinely solve high-resolution crystal structures without the need to grow large crystals is very appealing. Despite MicroED's exciting potential, adoption across the pharmaceutical industry has been slow, primarily owing to a lack of access to specialized equipment and expertise. Here we will present our experience building a small molecule MicroED service pipeline for members of the pharmaceutical industry. In the past year, we have examined more than fifty small molecule samples submitted by our clients, the majority of which have yielded data suitable for structure solution. We will also detail our experience determining small molecule MicroED structures of pharmaceutical interest and offer some insights into the typical experimental outcomes. This experience has led us to conclude thatsmall molecule MicroED adoption will continue to grow within the pharmaceutical industry where it is able to rapidly provide structures inaccessible by other methods.



