AutoMicroED: A semi-automated MicroED processing pipeline

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Microcrystal electron diffraction (MicroED) is a powerful but still relatively new cryogenic electron microscopy technique for atomic structure determination from three-dimensional crystals. Although there are many similarities between X-ray crystallography and MicroED, processing methods for MicroED data are not yet user friendly and widely distributed like they are in X-ray crystallography. While a few software suites exist to process MicroED data, there are currently no cohesive pipelines to semi-automatically process MicroED data with minimal user input. Instead, most users resort to piecing together and adapting software meant for processing X-ray crystallography data into a usable home-built package. This creates a bottleneck in structure elucidation and presents difficulties for novices in the field who may be new to both electron microscopy and dataset analysis. Here, we present AutoMicroED, a semi-automated pipeline for processing MicroED data. While this pipeline still leverages XDS, SHELX and other X-ray crystallography packages, it is bundled into a single installer and the entire process from indexing through phasing and structure solution can be run with a single command line call. Users can let the analysis run completely on its own, or users can engage flags that trigger quality check stops where the system stops and waits for the user to confirm indexing or other steps ran properly. Here we detail and demonstrate the AutoMicroED pipeline. We highlight several structures of standard small molecules with results comparable to that of their corresponding manually processed data. AutoMicroED is a useful processing tool for those new to the field of MicroED and will allow for faster and more efficient structure elucidation for both novice and experienced users.