

Using 10⁹ Molecules and a Synchrotron to Determine a Crystal Structure.

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We have collected x-ray diffraction intensity data on a single crystal of dimensions less than 10×40×40 microns at APS beamline 14-BM-C to 1Å. The space group is P2₁2₁2₁, and the cell dimensions are 7.8×13.0×46.7Å, with two independent molecules in the asymmetric unit at 100K. The molecules are natural products of pharmacological interest from the leaves and stems of *Solanum altissimum*, isolated as part of a collaborative research program to discover and evaluate novel cancer chemopreventive agents from plants. We were unable to obtain larger crystalline samples.

The structure was difficult to solve by direct methods, but several parallel approaches with SHELXS yielded all the non-hydrogen atoms. The structure refined to R=5.50% and GOF=1.25 with SHELXL (Sheldrick, 1990) without difficulty. Details on the data collection and processing of the intensity data will be presented. Suggestions for small molecule data collection at a synchrotron site will be included in the presentation.

