

## **Cannabidiol: A natural product structure in the mid-1970's. Weissenberg photos, four-circle diffractometry, direct methods, and more**

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The title compound, with formula C<sub>21</sub>H<sub>30</sub>O<sub>2</sub>, is a natural product whose absolute configuration was already known at the time the structure analysis was undertaken. The structure was analyzed in 1976 and published in 1977.[1] The analysis began with preliminary examination (today's pre-experiment) by Weissenberg photography, which yielded the cell dimensions and extinction symbol, which together with the fact that the compound was enantiomerically pure permitted an unambiguous determination of the space group. Intensity data were gathered using a semi-automated four-circle diffractometer (Syntex P21), measuring one complete, symmetry-unique sector of reciprocal space. Structure solution was by direct methods, and for this structure the starting set of reflections had to be defined by the user. Refinement was conducted using a new program with free-format input and easy calculation of hydrogen-atom positions. Calculations were done using an IBM370/165 with OS/MVT. The use of program overlay permitted the least-squares calculations to run in 128 K of computer memory. Some aspects of publication in this era will also be discussed. It is noted that more accurate analyses of this structure have been published in recent years.[2-4],