MS32-P11 | SOLID STATE STRUCTURE OF PHARMACEUTICALLY IMPORTANT COUMARIN DERIVATIVES FROM IN HOUSE COLLECTED XRPD DATA

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O-heterocycles show biological activities and coumarin derivatives are known as active pharmaceutical ingredients (APIs) and as antioxidants. Acenocoumarol is an anticoagulant Vitamin K antagonist. Pharmaceutical companies are relentlessly interested in the solid state structure of APIs as they are formed, *i.e*. as powders. Structure determination from X-ray powder diffraction pattern is more difficult than extracting structure from single crystal data (SCXRD). The main problem of this method, often called *ab initio* structure determination, is the inherent loss of data compared to SCXRD. Fortunately, modern X-ray sources, detectors and software resources open new possibilities to solve such difficult problems even using *in house* collected powder diffraction data and minimal sample manipulation. Powder patterns were collected using a Bruker D8 Venture diffractometer equipped with Photon II detector and dual (Mo and Cu) INCOATEC IμS 3.0 microsource using Cu Kα radiation. The sample was acenocoumarol powder. After indexing it turned out, that the unit cell dimensions are highly unusual, one unit cell axis was rather long. Use of the DASH package, part of the CSD software made it possible to index and integrate the pattern as well as solve and refine the structure. The results suggests, that intramolecular nucleophile addition occurred and a new derivative was formed. By extending the methodology compounds of similar chemical structures such as Trolox were also investigated. Analysis of non covalent interactions will also be reported.

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