Crystal structure of abiraterone acetate (Zytiga), $C_{26}H_{33}NO_2$

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Abiraterone acetate (trade name: Zytiga) is a prodrug used, in combination with prednisone, for the treatment of prostate cancer. Commercial abiraterone acetate crystallizes in the orthorhombic space group $P2_12_12_1$ with $a = 7.525265$ (14), $b = 9.733111(16)$, $c = 30.22909(10)$ Å, $V = 2214.106(7)$ Å^3, and $Z = 4$. A reduced cell search in the Cambridge Structural Database (Groom *et al*., 2016) yielded a previously reported crystal structure (Zhou *et al*., 2015) collected at 283 K. In this work, the sample was ordered from Carbosynth and analyzed as received. The room-temperature crystal structure was refined using synchrotron ($\lambda = 0.413691$ Å) powder diffraction data, density functional theory, and Rietveld refinement techniques. The diffraction data were collected on beamline 11-BM at the Advanced Photon Source, Argonne National Laboratory. Figure 1 shows the powder X-ray diffraction pattern of the compound. The crystal structure is dominated by van der Waals interactions and electrostatic forces. There are no hydrogen bonds. The pattern is included in the Powder Diffraction File as entry 00-065-1409.

SUPPLEMENTARY MATERIAL

The supplementary material for this article can be found at https://doi.org/10.1017/S0885715618000015.

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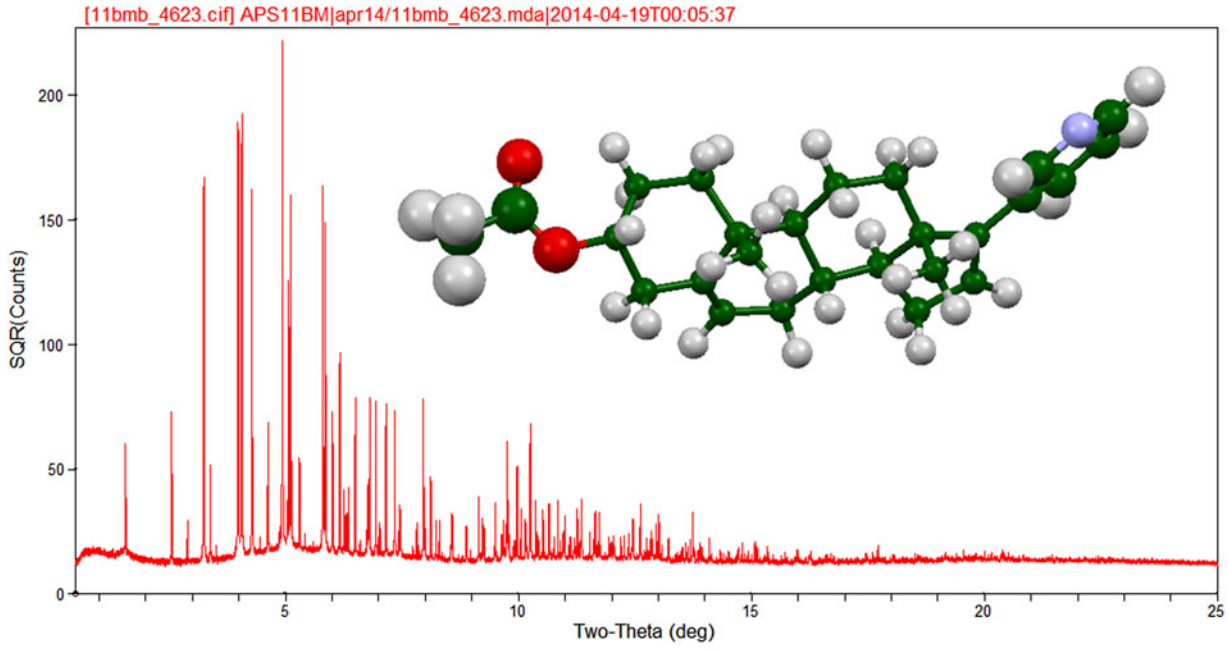

Figure 1. (Color online) Powder X-ray diffraction pattern of abiraterone acetate.

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