Crystal structure of estradiol 17β valerate (Delestrogen), $C_{23}H_{32}O_3$

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Estradiol valerate (brand name: Delestrogen) is used as a hormone replacement therapy for menopause symptoms and for treating advanced prostate cancer. Commercial estradiol 17β valerate crystallizes in the monoclinic space group $P2_1$ with $a = 7.36787(3)$, $b = 19.84900(6)$, $c = 13.99395(10)$ Å, $\beta = 90.6845(5)°$, $V = 2046.398(18)$ Å^3, and $Z = 4$. © *2018 International Centre for Diffraction Data.*
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Key words: estradiol valerate, powder diffraction, Rietveld refinement, density functional theory

Estradiol valerate (brand name: Delestrogen) is used as a hormone replacement therapy for menopause symptoms and for treating advanced prostate cancer. Commercial estradiol 17β valerate crystallizes in the monoclinic space group $P2_1$ with $a = 7.36787(3)$, $b = 19.84900(6)$, $c = 13.99395(10)$ Å, $\beta = 90.6845(5)°$, $V = 2046.398(18)$ Å^3, and $Z = 4$. A reduced cell search in the Cambridge Structural Database (Groom *et al.*, 2016) yielded a previously reported crystal structure above 251 K (Ellena *et al.*, 2014). In this work, the sample was ordered from U.S. Pharmacopeial Convention (USP), Lot #M0M476 and analyzed as received. The room-temperature crystal structure was refined using synchrotron ($\lambda = 0.414163$ 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 contains two independent chains of O–H• • • O hydrogen bonds along the *c*-axis. Weak C–H• • • O hydrogen bonds also contribute to the crystal energy. The conformation of the

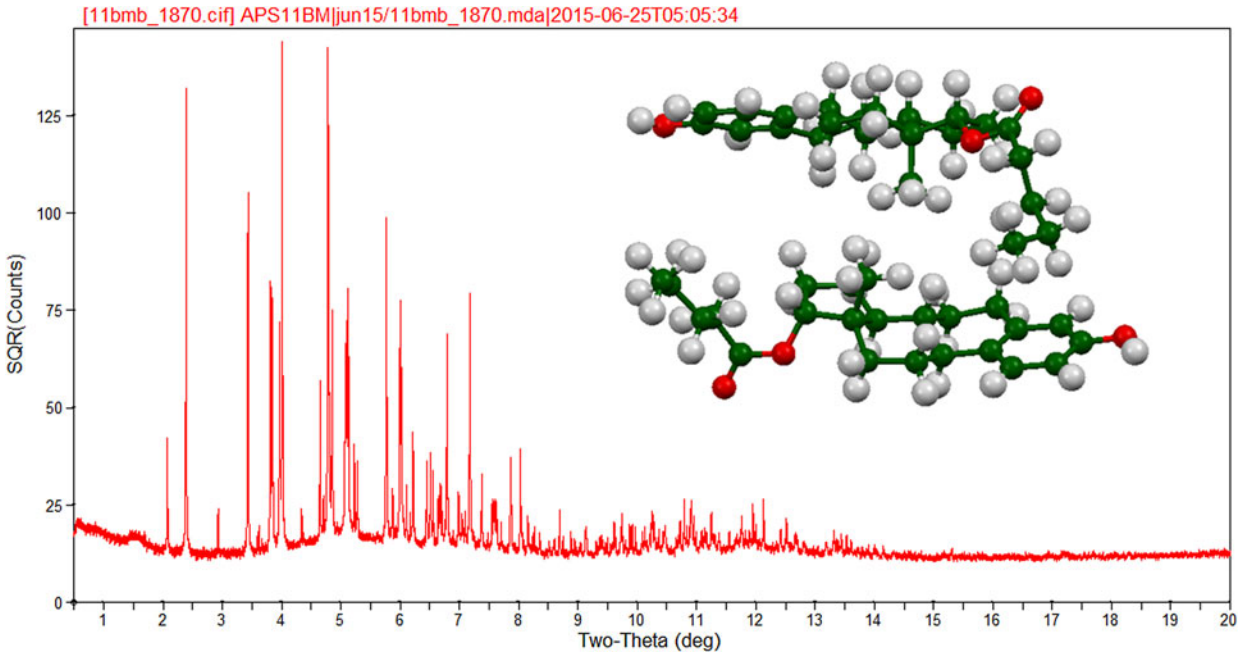

Figure 1. (Colour online) Powder X-ray diffraction pattern of estradiol 17β valerate.

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valerate side chain in one molecule (C46–C51) differs from that reported by Ellena *et al*. (2014). The pattern is included in the Powder Diffraction File as entry 00-066-1612.

SUPPLEMENTARY MATERIAL

The supplementary material for this article can be found at https://doi.org/10.1017/S0885715618000039.

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