Powder X-ray diffraction of 1-(4-aminophenyl)-5,6-dihydro-3-(4-morpholinyl)-2(1H)-pyridinone, $C_{15}H_{19}N_3O_2$

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X-ray powder diffraction data for 1-(4-aminophenyl)-5,6-dihydro-3-(4-morpholinyl)-2(1H)-pyridinone, $C_{15}H_{19}N_3O_2$, are reported [$a = 14.877(4)$ Å, $b = 5.893(6)$ Å, $c = 18.984(3)$ Å, $\alpha = 90°$, $\beta = 122.298(3)°$, $\gamma = 90°$, unit-cell volume $V = 1406.86$ Å^3, $Z = 4$, and space group $P2_1/c$]. All measured lines were indexed and are consistent with the $P2_1/c$ space group. No detectable impurities were observed. © *2015 International Centre for Diffraction Data*. [doi:10.1017/S088571561500072X]

Key words: 1-(4-aminophenyl)-5,6-dihydro-3-(4-morpholinyl)-2(1H)-pyridinone, pharmaceutical intermediate, anticoagulant, apixaban

1-(4-aminophenyl)-5,6-dihydro-3-(4-morpholinyl)-2(1H)-pyridinone is an intermediate in the synthesis of the anticoagulant, Apixaban (Watson *et al*., 2011; Jiang and Ji, 2013). The sample was prepared using 3-(4-morpholinyl)-1-(4-nitrophenyl)-5,6-dihydro-2(1H)-pyridinone and was recrystallized in methanol and dried. The sample was then ground into powder (HPLC ≥ 98%, $\rho = 1.283$ g cm^{-3}, T_{melt} = 180–182 °C) and mounted on a flat zero background plate. X-ray powder diffraction measurement was performed at room temperature using an X'Pert PRO diffractometer (PANalytical Co., Ltd., The Netherlands) with a PIXcel 1D detector and Cu$K\alpha$ radiation (generator setting: 40 kV and 40 mA). The diffraction data were collected over the angular range from 4° to 50°2θ with a step size of 0.013 13°2θ and a counting time of 30 ms step^{-1}. The software package Material Studio 8.0 (Accelrys Co., Ltd., CA, USA) was used to process the data in the Analytical & Testing Center (Sichuan University, China). The X-ray powder diffraction pattern was pre-treated by subtracting the background, smoothing, and stripping off the $K\alpha_2$ component. Automatic indexing results were obtained by X-Cell method (Neumann, 2003). The preliminary cell from indexing was refined using the Pawley method (Pawley, 1981). The refinement confirmed that the sample crystallizes in the monoclinic space group $P2_1/c$ (14), with $a = 14.877(4)$ Å, $b = 5.893(6)$ Å, $c = 18.984(3)$ Å, $\alpha = 90°$, $\beta = 122.298(3)°$, $\gamma = 90°$, $V = 1406.86$ Å^3, $Z = 4$, and $\rho_x = 1.290$ g cm^{-3}. Figure 1 shows the Powder X-ray diffraction pattern of the compound.

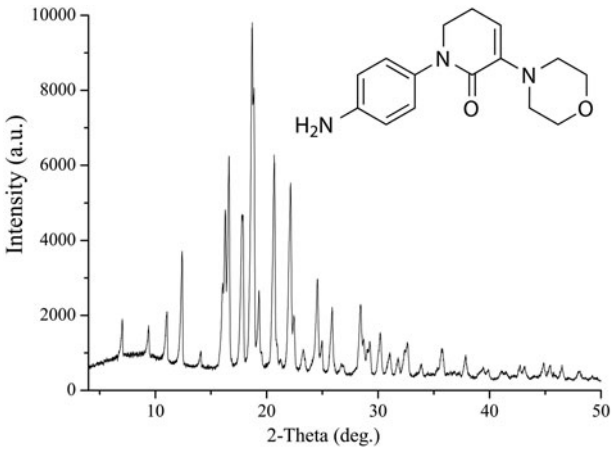

Figure 1. Powder X-ray diffraction pattern of the compound.

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SUPPLEMENTARY MATERIALS AND METHODS

The supplementary material for this article, can be found at http://dx.doi.org/10.1017/S088571561500072X

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