Powder X-ray diffraction of bendamustine hydrochloride monohydrate, $C_{16}H_{22}Cl_2N_3O_2Cl \cdot H_2O$

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Bendamustine hydrochloride monohydrate (marketed as Treanda®) is a nitrogen mustard purine analog alkylator used in the treatment of chronic lymphocytic leukemia (CLL) and non-Hodgkin lymphomas. Commercial bendamustine hydrochloride monohydrate crystallizes in the monoclinic space group $P2_1/c$ (14), with $a = 4.71348(4)$ Å, $b = 47.5325(3)$ Å, $c = 8.97458$ (5) Å, $\beta = 96.6515(8)°$, $V = 1997.161(23)$ Å^3, and $Z = 4$. A reduced cell search in the Cambridge Structural Database yielded a previously reported crystal structure (Allen, 2002), which did not include hydrogens (Reck, 2006). In this work, the sample was ordered from Santa Cruz Biotechnology, and analyzed as received. The room-temperature crystal structure was refined using synchrotron ($\lambda = 0.413896$ Å) powder diffraction data, density functional theory (DFT), and Rietveld refinement techniques. Hydrogen positions were included as part of the structure, and recalculated during the refinement. The diffraction data were collected on beamline BM-11 at the Advanced Photon Source, Argonne National Laboratory. Figure 1 shows the powder X-ray diffraction pattern of the compound. The pattern is included in the Powder Diffraction File as entry 00-064-1508.

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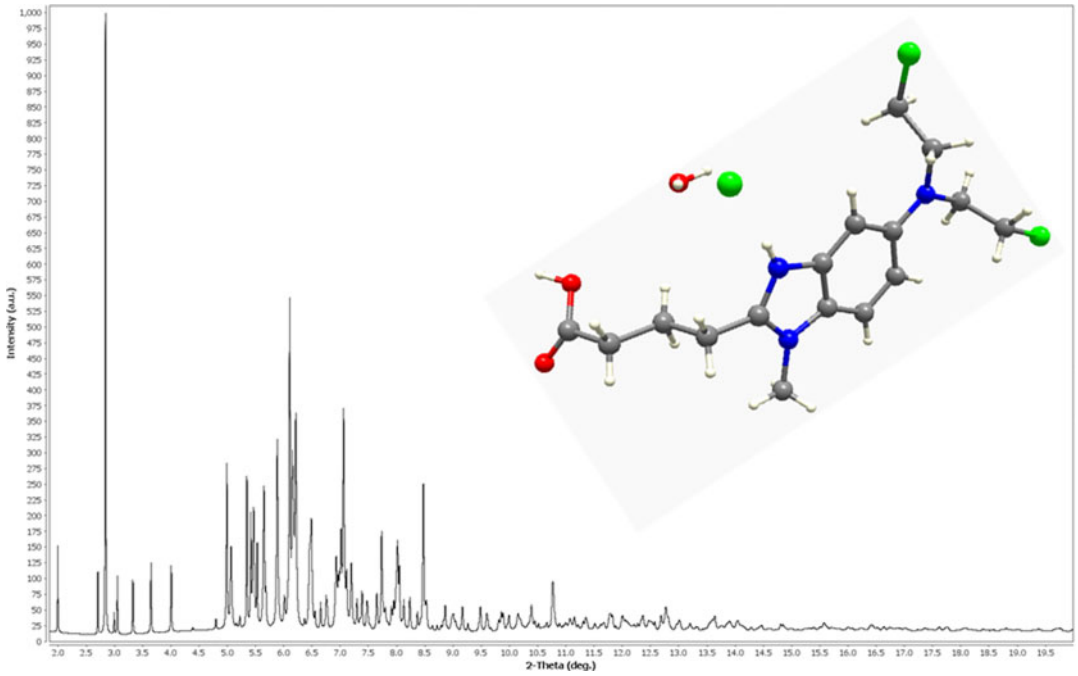

Figure 1. (Color Online) Powder X-ray diffraction pattern of bendamustine hydrochloride monohydrate.

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SUPPLEMENTARY MATERIAL

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