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### **Solid State Characteristics of Bedaquiline Benzoate**

Bedaquiline was approved for the treatment of multi-drug-resistant tuberculosis in 2012. Understanding the solid-state properties of the benzoate salt opens potentials for manufacturing it as a new molecular entity. There has been some communications on crystal salts of bedaquiline; this work provides more insight to the characterisation for the benzoate salt. The salt was formed from 1:1 ratio of 30mg (0.054 millimoles) bedaquiline and the millimole equivalents, 6.6mg of benzoic acid. Single crystal structures were determined at 150 K using Bruker Quest X-ray diffractometers using either Mo K( $\lambda = 0.71073 \text{ \AA}$ ) or Cu K radiation ( $\lambda = 1.54178 \text{ \AA}$ ). The sample was analysed by PXRD, and the structure confirmed by Rietveld analysis against the single crystal. Sorption potentials for the salt was determined at 75% and 0% relative humidities (RH), while accelerated stability was conducted at 40°C and 75% RH. Thermal analysis was conducted using melting point, DSC, and TGA. Water content of the hydrate benzoate was by KF titrations. Bedaquiline benzoate occurs as a monocation protonated selectively at the dimethyl amine substituent., the less basic quinoline N atoms remains unprotonated. It occurs as either a 1.17 hydrate or a monohydrate acetonitrile solvate. The chemical formula was  $C_{32}H_{32}BrN_2O_2 \cdot C_7H_5O_2 \cdot 1.166(H_2O)$ , Mwt 698.7g. Rietveld analysis confirmed the benzoate salts. The DSC thermographs value was comparable to the melting point determination. KF determination shows it contained 3.33% water, comparable to the TGA results, loss of ~3.1%. The salt was stable and non-hygroscopic (<0.1% weight gain) at ambient conditions for > 3 months.

### **Biography**

Mercy Okezue is a Ph.D. candidate in the [Biotechnology Innovation and Regulatory Science \(BIRS\)](#) program at Purdue University, West Lafayette, IN. Simultaneously, she works as a regulatory officer with Nigeria's foods and drugs regulatory authority, NAFDAC. A fellow of the West African Post-Graduate College of Pharmacists (2010), Pharm. Okezue also has an MS degree in BIRS from Purdue (2016). Currently, she is a teaching fellow in Purdue University BIRS M.S. program and also researches advancing solutions in the pharmaceutical quality control space. She works in Prof. Stephen Byrn's lab and is currently characterizing five novel salts of bedaquiline; a drug for treating multi-resistant tuberculosis.



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