CHARACTERIZATION OF PHARMACEUTICALS BY XRPD AND THERMAL ANALYSIS: BUPROPION HYDROCHLORIDE

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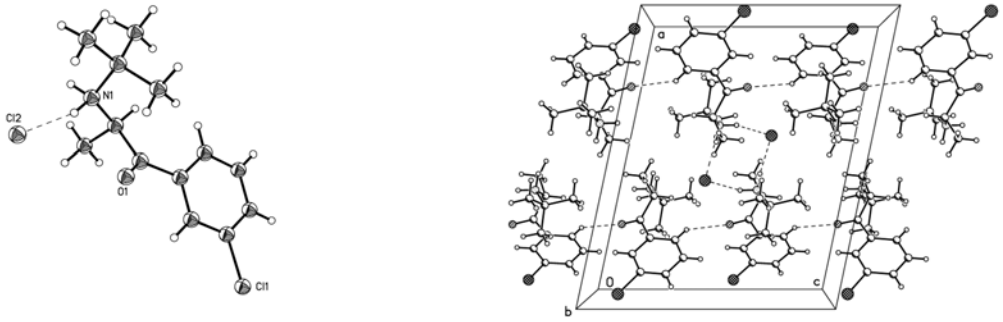
The results presented here come from a joint project between academia and Italian pharmaceutical industries. In our recent studies [1], the structural models of Dehydrocholic Acid, Acitretin, Linezolid, Sibutramine, and Azelastine were obtained by laboratory powder diffraction data only and were further corroborated by TG, DSC and thermodiffractometric analyses, as well as by ^{13}C solid state NMR measurements. The characterization of such polycrystalline phases of pharmaceutical interest (thermal generated polymorphs, metastable anhydrous species, solvates, etc.) was favored by the development of a relevant methodology, the availability of computer programs allowing real-space structural solutions and the use (during the simulated annealing and Rietveld refinements steps) of flexible models of known connectivity.
We present here the complete structure characterization and the crystal chemistry of Bupropion hydrochloride, a second generation antidepressant, the molecular and crystal structure of which are shown below.



[1] See for example: Maccaroni, E., Alberti, E., Malpezzi, L., Masciocchi, N., Vladiskovic, C. 2008. *Int. J. Pharm.* 351, 144-151; Maccaroni, E., Alberti, E., Malpezzi, L., Masciocchi, N., Pellegatta, C. 2008. *J. Pharm. Sci.* 97, 5229-5239; E. Maccaroni, E. Alberti, L. Malpezzi, G. Razzetti, C. Vladiskovic, N. Masciocchi, *Cryst. Growth Des.*, 9, 517-524 (2009).