

Poster Presentation

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Phase transitions in efavirenz induced by mechanical activation

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Efavirenz, (S)-6-chloro-4(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)-2H-3,1-benzoxazin-2-one, is a anti HIV agent belonging to the class of the non-nucleoside reverse transcriptase inhibitors, which is used in combination with other protease inhibitors or nucleoside reverse transcriptase inhibitors. Several polymorphs were reported in patents and scientific publications, being form I the thermodynamically most stable and the selected for commercial formulations. Mechanochemistry has emerged as an experimental methodology to efficiently and rapidly screen for new solid forms of a pharmaceutical active ingredient. These methods include neat and drop assisted grinding have been successfully applied to produce solvates, polymorphs, salts and cocrystals. In this contribution, we investigate the structural stability of efavirenz under mechanochemistry conditions. Room temperature and cryogenic neat and drop assisted grinding were applied to induce new crystalline forms, which were characterized by x-ray powder diffraction, vibrational spectroscopy and thermal analysis. The mechanism involved in these transformations were also investigated and discussed.

Keywords: Efavirenz, Ball milling, Phase transitions