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Title:	New Polymorphs of Fluconazole: Results from Cocrystallization Experiments
Authors:	Karanam, M. (/jspui/browse?type=author&value=Karanam%2C+M.) Dev, Sagarika (/jspui/browse?type=author&value=Dev%2C+Sagarika) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	X-ray diffraction
Issue Date:	2012
Publisher:	American Chemical Society.
Citation:	Crystal Growth & Design, 12(1), 240-252 .
Abstract:	Fluconazole is known as an antifungal drug since 1983. Its propensity for the formation of new polymorphs and salts has been reported in the literature, mostly by powder X-ray diffraction and solid state Raman spectroscopy. In the present study, we are elucidating the structures of four polymorphs of fluconazole using single crystal X-ray diffraction. Raman spectra of the single crystals of these polymorphs also support our study. These polymorphs were grown in the presence of the cocrystal formers. This indicates that fluconazole interacts with the cocrystal former in the solution, and possibly these interactions result into the generation of new polymorphs of it. These polymorphs of fluconazole exhibit the conformational flexibility of the molecule, and hence we observed seven different conformers of the molecule in the reported polymorphs. Although these forms have strong O-H...N hydrogen bonds, the nature of the packing of the molecules is a cumulative effect of a number of weaker intermolecular forces such as C-H...O, C-H...N, and C-H...F and the strong hydrogen bond.
URI:	http://pubs.acs.org/doi/full/10.1021/cg201005y (http://pubs.acs.org/doi/full/10.1021/cg201005y)
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