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Title: The evaluation of the role of C–H...F hydrogen bonds in crystal altering the packing modes in the presence of strong hydrogen bond

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Abstract: Interactions involving fluorine is an area of contemporary research. To unravel the importance of weak C–H...F hydrogen bonds and C–H... π interactions in organic compounds in the presence of strong hydrogen bond, a series of N-benzylideneanilines with simultaneously hydroxyl (–OH) and fluorine substitutions were synthesized for structural analysis. These compounds have been studied through experimental single crystal X-ray diffraction analysis and computational methods (Gaussian09 and AIM2000). The hydroxyl group present in all the molecules were found to form strong O–H...N hydrogen bond, but the spatial arrangement of the molecules connected by this hydrogen bond have been found to be controlled by the weak C–H...F and C–H...O hydrogen bonds, weak C–H... π and π ... π interactions. This manuscript illustrates the importance of several weaker interactions in altering the packing modes in the presence of strong hydrogen bonds.

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