Poster Presentation

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Experimental and computational insights into energy contributions of intermolecular interactions

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The presence of the C–F bond in organic molecules, particularly in the context of generating different intermolecular interactions of the type C–F•••F–C, C–H•••F–C and C–F•••π is of extreme significance in the realm of structural chemistry [1]. These interactions generate different packing motifs in the formation of the crystal. It is of interest to evaluate the energetic contributions of such weak interactions to evaluate their important role in crystal packing [2]. In this respect, a library of nine compounds containing a strong donor(N–H) and a strong acceptor(C=O), along with the presence of C–F bonds in different phenyl rings have been synthesized and these have been characterized using 1H NMR, single crystal, and powder X-ray diffraction techniques and their melting points were determined by DSC. In addition, the non-fluorinated counterpart has also been synthesized & characterized. A plethora of weak interactions, namely aromatic C(sp2)H•••F-C(sp2), aliphatic C(sp2)H•••F-C(sp2), C(sp2)-F•••F-C(sp2) and C(sp2)-F•••π are involved in crystal packing in the presence of strong N-H•••O=C hydrogen bonds [3] and π•••π contacts [4]. Detailed analyses of all the crystalline solids were performed with quantitative inputs from interaction energy calculations using the PIXEL method and a complete topological analyses were used to characterize these interactions.

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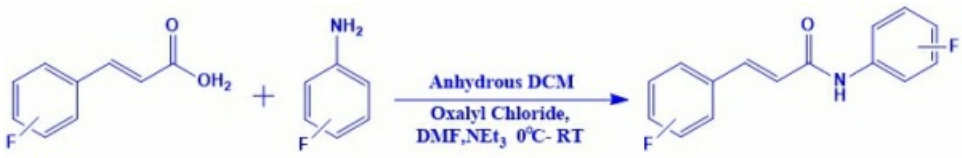

Figure 1: Synthesis of fluorine substituted 3-phenyl-N-phenyl-2-propenamides from fluoro substituted cinnamic acids & anilines.

Keywords: Intermolecular Interactions, Flourine, Crystal Packing