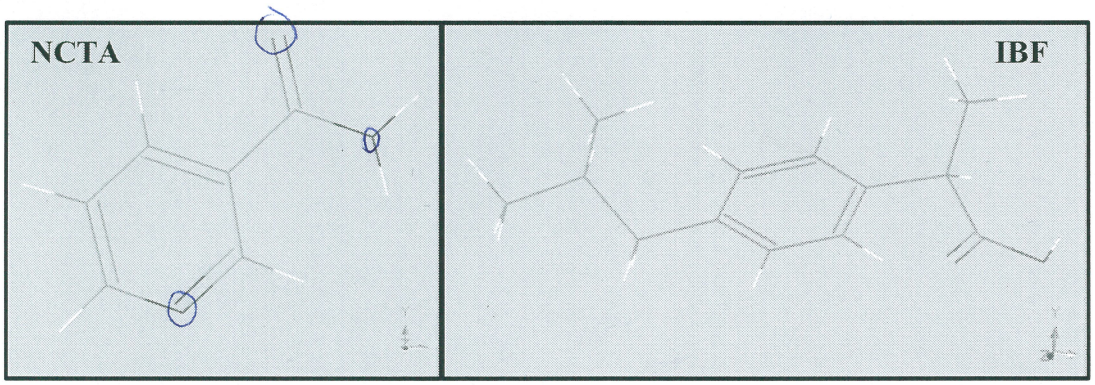

Fig. 1. Relaxed structure of ibuprofen (IBF) and nicotinamide (NCTA) calculated using DFT.

The calculated sigma charge densities of IBF and NCTA are reported in Fig. 2. For both IBF and NCTA, significant peaks have been observed within the nonpolar region i.e. $-0.01<\sigma<0.01$ e/Å^2. This means that most of the surface of these molecules has nonpolar characteristics. In NCTA, the peak around $\sigma = -0.014$ e/Å^2 is due to the two polarized hydrogen atoms bounded to nitrogen atom. The peak around $\sigma = -0.006$ e/Å^2 is due to hydrogens available in ring. The peak around $\sigma = 0.002$ e/Å^2 is due to exposed surfaces of carbon atoms. The peak around $\sigma = 0.014$ e/Å^2 is due to the lone-electrons on oxygen in C=O group. The peak around $\sigma = 0.009$ e/Å^2 is due to lone-electron on nitrogen in ring and NH_2 group. The peak around $\sigma = -0.003$ e/Å^2 is due CH groups.

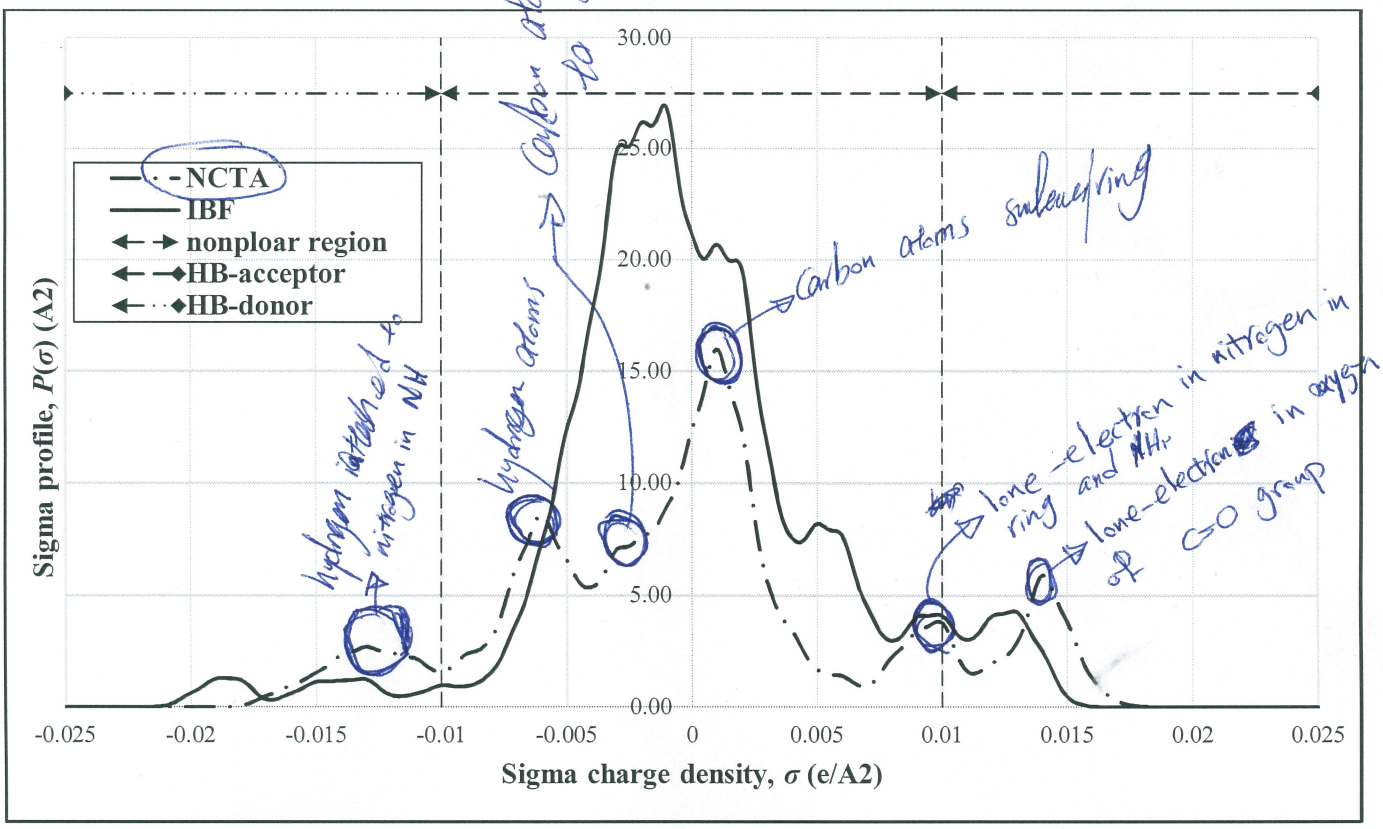

Fig. 2. Sigma charge densities of ibuprofen (IBF) and nicotinamide (NCTA) calculated using DFT/cosmo.