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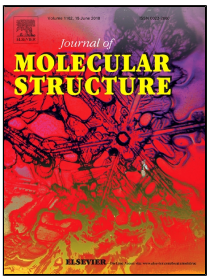

XPS investigation of new solid forms of 5-fluorouracil with piperazine

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XPS investigation of new solid forms of 5-fluorouracil with piperazine

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Abstract

The present study reports the results obtained by X-ray photoelectron spectroscopy (XPS) for new solid forms of antineoplastic agent 5-fluorouracil with anthelmintic piperazine obtained by liquid assisted ball milling and slurry crystallization methods as co-crystal and salt, respectively. The interest for these new solid forms of 5-fluorouracil with onother drug consists in obtaining new compounds with potential pharmaceutical and biomedical applications. The XPS results bring additional deciding information on the atomic environments in the newly obtained solid forms of 5-fluorouracil with piperazine beside the earlier reported X-ray diffraction and infrared spectroscopy data. The deconvolution of N 1s core level spectra allows to distinguish unequivocally the protonated (salt) from hydrogen-bonded (co-crystal) nitrogen species based on the N 1s binding energy associated with the protonation of nitrogen atoms. The N 1s component around 402 eV observed only for the solid form obtained following the slurry route proves in this case the formation of a salt on basis of positively charged nitrogen resulted by protonation of secondary amine groups. Moreover, for the solid form obtained following the ball milling route, one notices a large negative shift of N 1s binding energy that supports the development of a co-crystal.

Keywords*: 5-Fluorouracil; piperazine; co-crystal; salt; XPS.*

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