

SUPPORTING INFORMATION

Supramolecular Synthesis and Characterization of Crystalline Solids Obtained from the Reaction of 5-Fluorocytosine with Nitro Compounds

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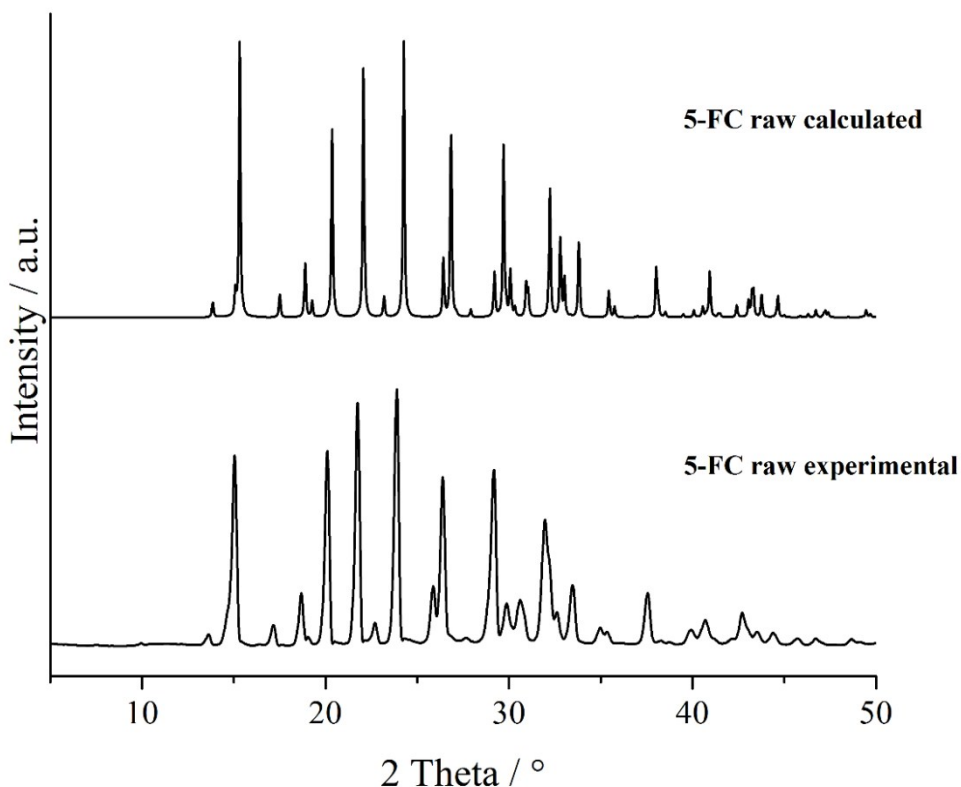


Figure S1. Calculated and experimental powder X-ray diffraction patterns of 5-Fluorocytosine. The diffraction patterns are in good agreement indicating that the starting material present high crystallinity and purity.

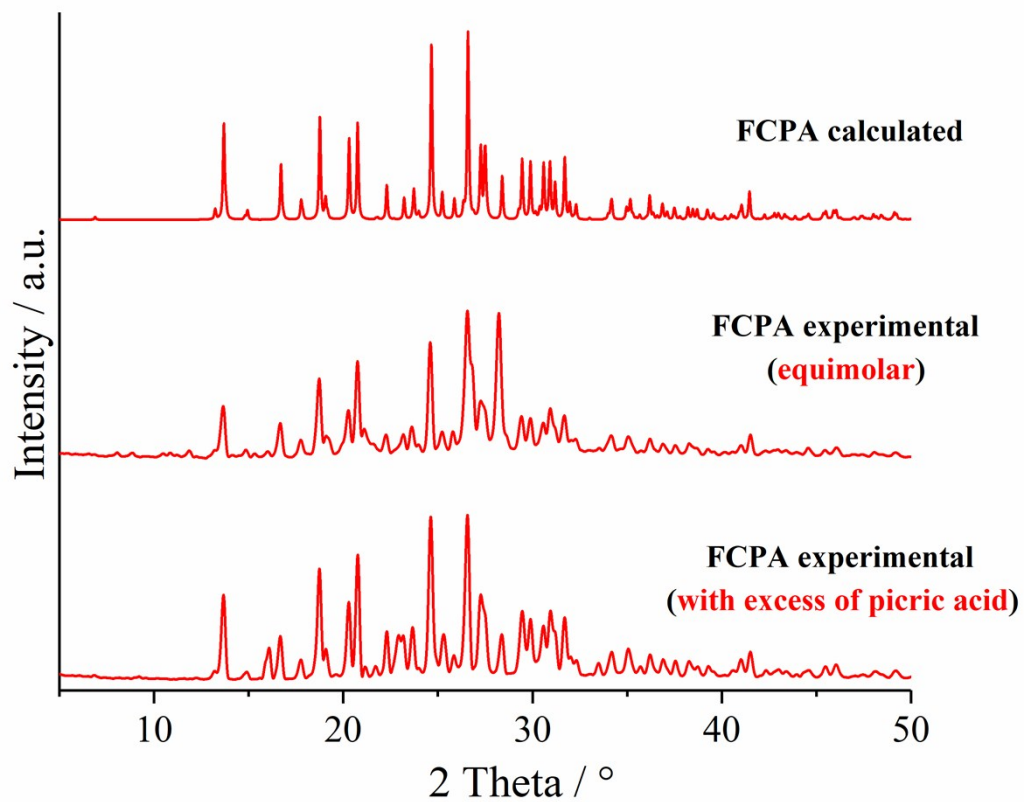


Figure S2. Calculated and experimental (in different stoichiometries) powder X-ray diffraction patterns of FCPA salt.

Table S1. Angular dimensions of protonated and neutral 5-Fluorocytosine.

Compound	(C2-N3-C4) internal angle / °
Neutral 5-FC	120.8(5)
FCPA	125.6(1)
2FCPA	125.0(2)
FCDNS	124.8(1)

Table S2. Calculated ΔpK_a values for the reaction of 5-FC with the nitro acids studied here.

Compound	pK_a	$\Delta pK_a = (pK_a(5-FC) - pK_a(acid))$
5-Fluorocytosine	3.26 ⁸	-
Picric acid	0.38 ³⁵	2.88
3,5-dinitrosalicylic acid	2.2 ⁵⁹	1.06

[^{8, 35, 59}] = References in the manuscript.