

## Supporting Information

### Supramolecular self-assembly and perfected *in vitro/vivo* property of 5-fluorouracil and ferulic acid on the strength of double optimized strategy: The first 5-fluorouracil-phenolic acid nutraceutical cocrystal with synergistic antitumor efficacy

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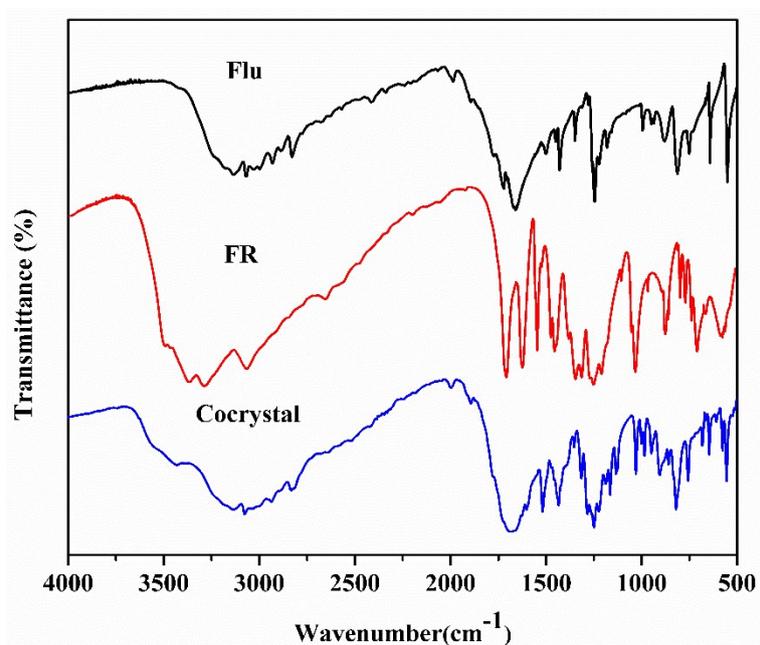
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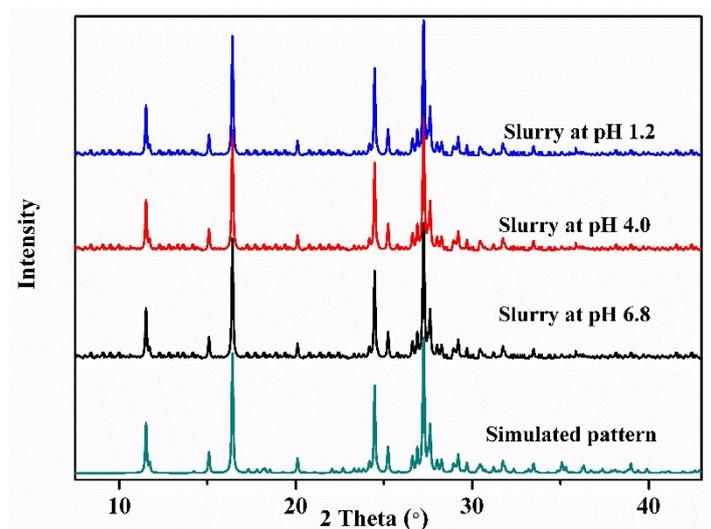
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**Table S1** The MEP around hydrogen bonding associated atoms in Flu and cocrystal

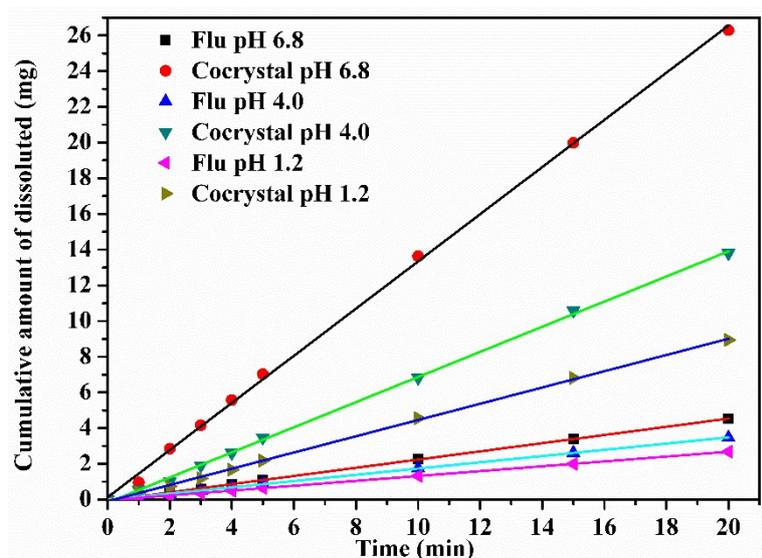
	a	b	c
O1	-12.27, -12.24	-25.57	
O2	-37.39, -37.40		42.03, -30.14
O3		-24.38	
O4		-20.16	
O5			
O7			-33.48, -52.88
H1	43.17, 43.19		10.21
H2A	40.60, 40.56	38.86	35.35
H3			7.43
H4		14.04	
H7A			43.77, 17.66
H7B			27.78, 2.82



**Fig. S1** FT-IR spectra of plain Flu and FR, together with Flu-FR-H<sub>2</sub>O cocrystal.



**Fig. S2** PXR D comparison of simulated pattern and experimental pattern for residual solids after the powder dissolution measurements.



**Fig. S3** IDR profiles of Flu and Flu-FR-H<sub>2</sub>O cocystal at pH 1.2, 4.0, and 6.8.