Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary data for

A 5-fluorouracil-kaempferol drug-drug cocrystal: ternary phase diagrams, characterization and property evaluation

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Table S1. Selected hydrogen bonding distances and angles for **5FU-KAE**.

Hydrogen bond	H···A (Å)	D···A (Å)	∠D−H···A (°)	symmetry code
N1−H1A···O4	1.9 35	2.753	158.40	-x+1/2, y-1/2, -z+1/2
N2−H2B···O1	2.055	2.897	166.08	x+1, y-1, z
O6−H6···O7	1.847	2.664	174.43	
O5−H5···O8	2.095	2.864	156.12	-x+1/2, y+1/2, -z+1/2
O1−H1···O6	1.891	2.700	168.43	-x+1/2, y+1/2, -z+3/2
O2−H2···O4	1.887	2.616	147.38	

Table S2. All points for the construction of a ternary phase diagram at 25 °C.

		5FU concentration (mol/L)	KAE concentration (mol/L)	EtOH concentration (mol/L)
Point 1	5FU	0.0259	0	0.9741
Point 2	5FU	0.0345	0.0192	0.9464
Point 3	5FU and **5FU-KAE**	0.0377	0.0192	0.9431
Point 4	5FU and **5FU-KAE**	0.0416	0.0179	0.9405
Point 5	5FU and **5FU-KAE**	0.0432	0.0171	0.9397
Point 6	5FU and **5FU-KAE**	0.0467	0.0177	0.9356
Point 7	**5FU-KAE**	0.0327	0.0244	0.9428
Point 8	**5FU-KAE**	0.0025	0.1965	0.8010
Point 9	KAE and **5FU-KAE**	0.0014	0.2739	0.7247
Point 10	KAE and **5FU-KAE**	0.0015	0.2943	0.7042
Point 11	KAE	0.0015	0.3058	0.6927
Point 12	KAE	0	0.3509	0.6491

Table S3. All points for the construction of a ternary phase diagram at 40 °C.

		5FU concentration (mol/L)	KAE concentration (mol/L)	EtOH concentration (mol/L)
Point 1	5FU	0.0364	0	0.9636
Point 2	5FU	0.0405	0.0291	0.9304
Point 3	5FU and **5FU-KAE**	0.0439	0.0284	0.9277
Point 4	5FU and **5FU-KAE**	0.0471	0.0265	0.9264
Point 5	5FU and **5FU-KAE**	0.0494	0.0290	0.9216
Point 6	5FU and **5FU-KAE**	0.0557	0.0265	0.9178
Point 7	**5FU-KAE**	0.0428	0.0305	0.9267
Point 8	**5FU-KAE**	0.0036	0.2936	0.7033
Point 9	KAE and **5FU-KAE**	0.0023	0.4047	0.5930
Point 10	KAE and **5FU-KAE**	0.0032	0.4130	0.5838
Point 11	KAE	0.0024	0.4350	0.5626
Point 12	KAE	0	0.4076	0.5924

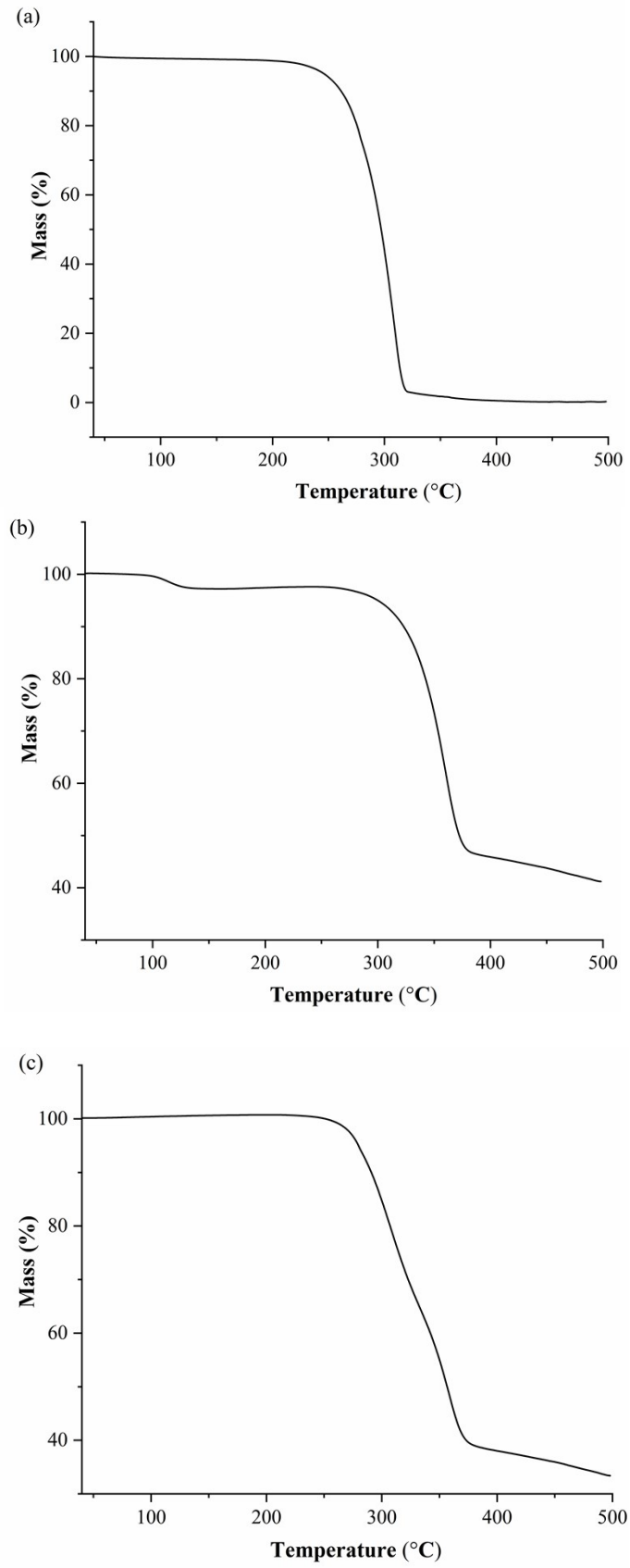

Fig. S1 TG thermograms of (a) 5FU, (b) KAE·0.5H_2O and (c) **5FU-KAE**.

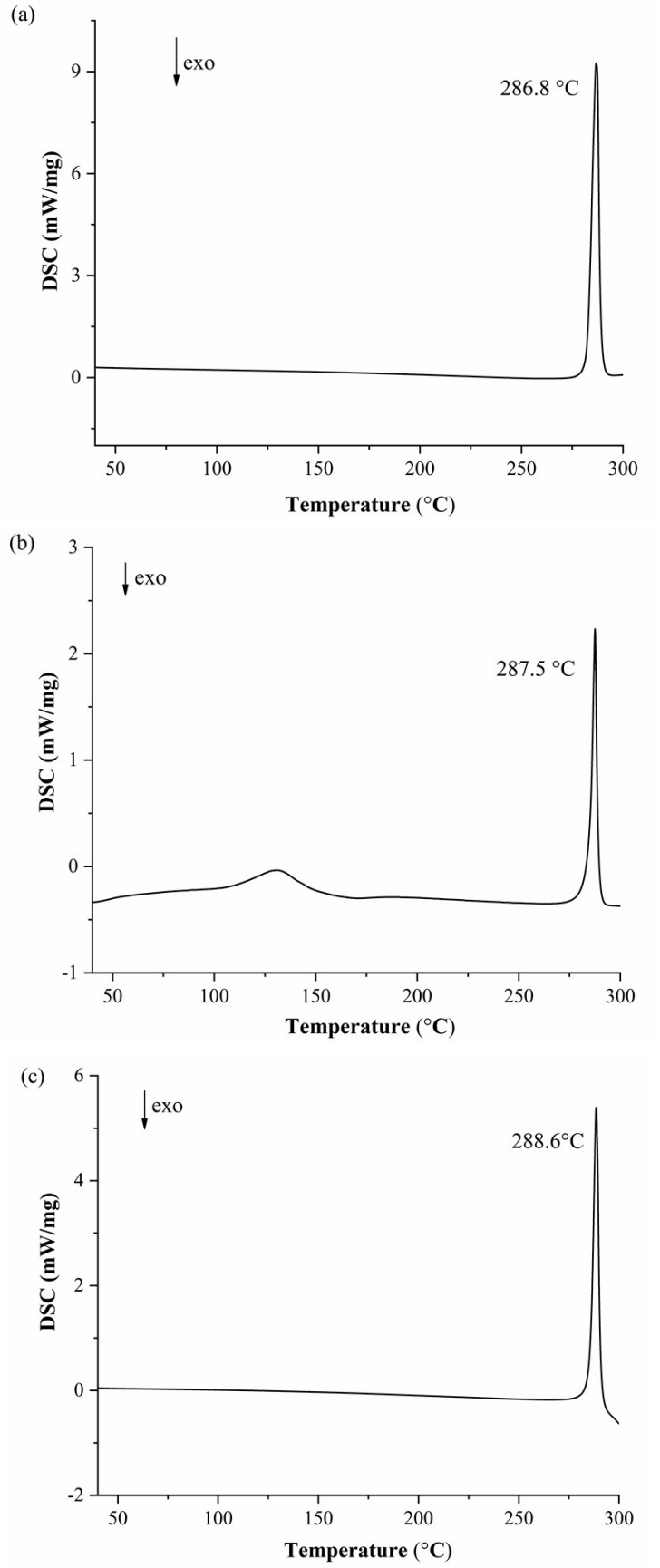

Fig. S2 DSC thermograms of (a) 5FU, (b) KAE·0.5H_2O and (c) **5FU-KAE**.

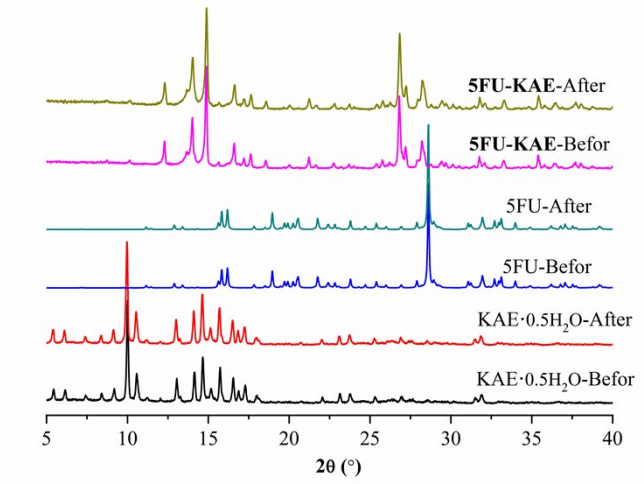

Fig. S3 PXRD patterns for 5FU, KAE·0.5H_2O and **5FU-KAE** before and after DVS.

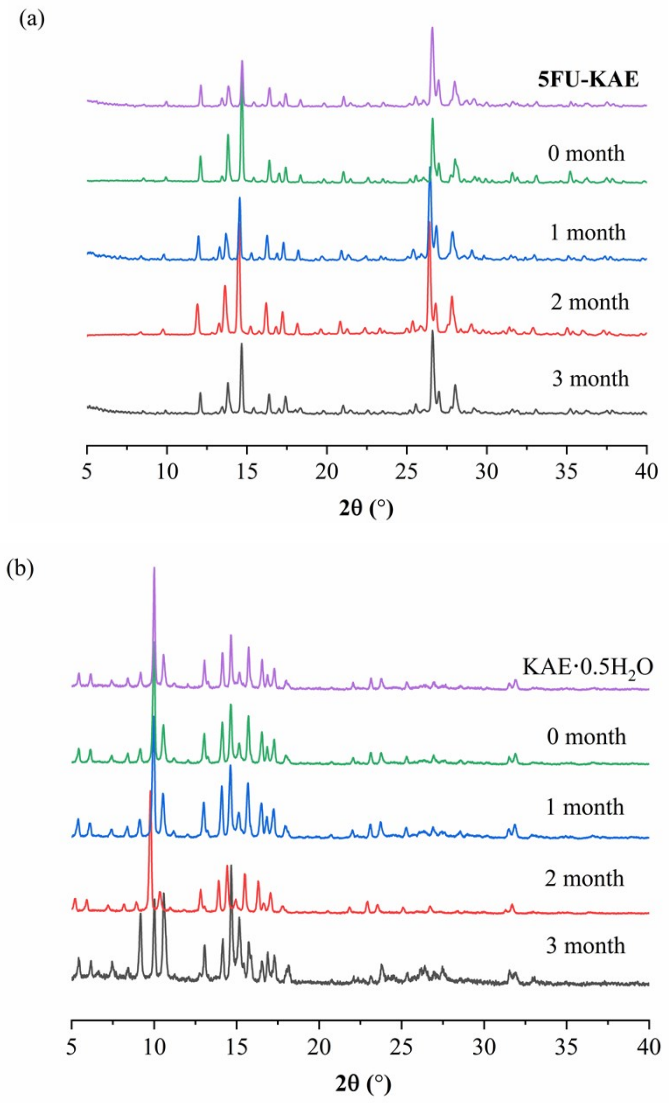

Fig. S4 PXRD patterns under accelerated conditions for (a) **5FU-KAE** and (b) KAE·0.5H_2O.

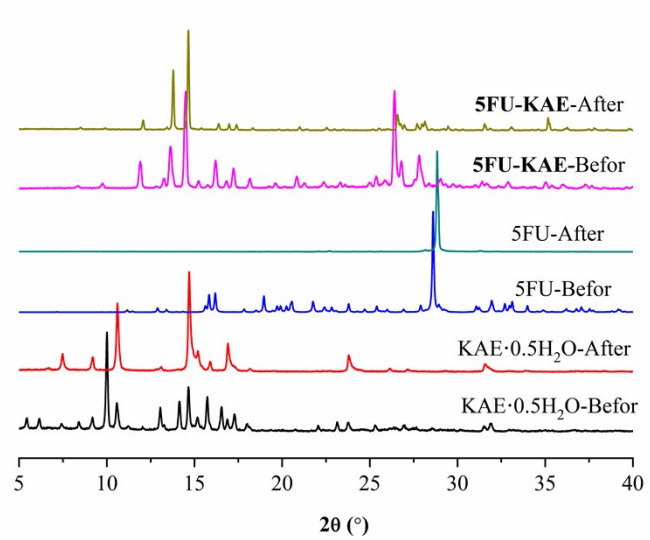

Fig. S5 PXRD patterns of 5FU, KAE·0.5H_2O and **5FU-KAE** after dissolution test.