

## Supplementary data for

### **Salts of rucaparib with dicarboxylic acids: synthesis, crystal structures and solubility aspects**

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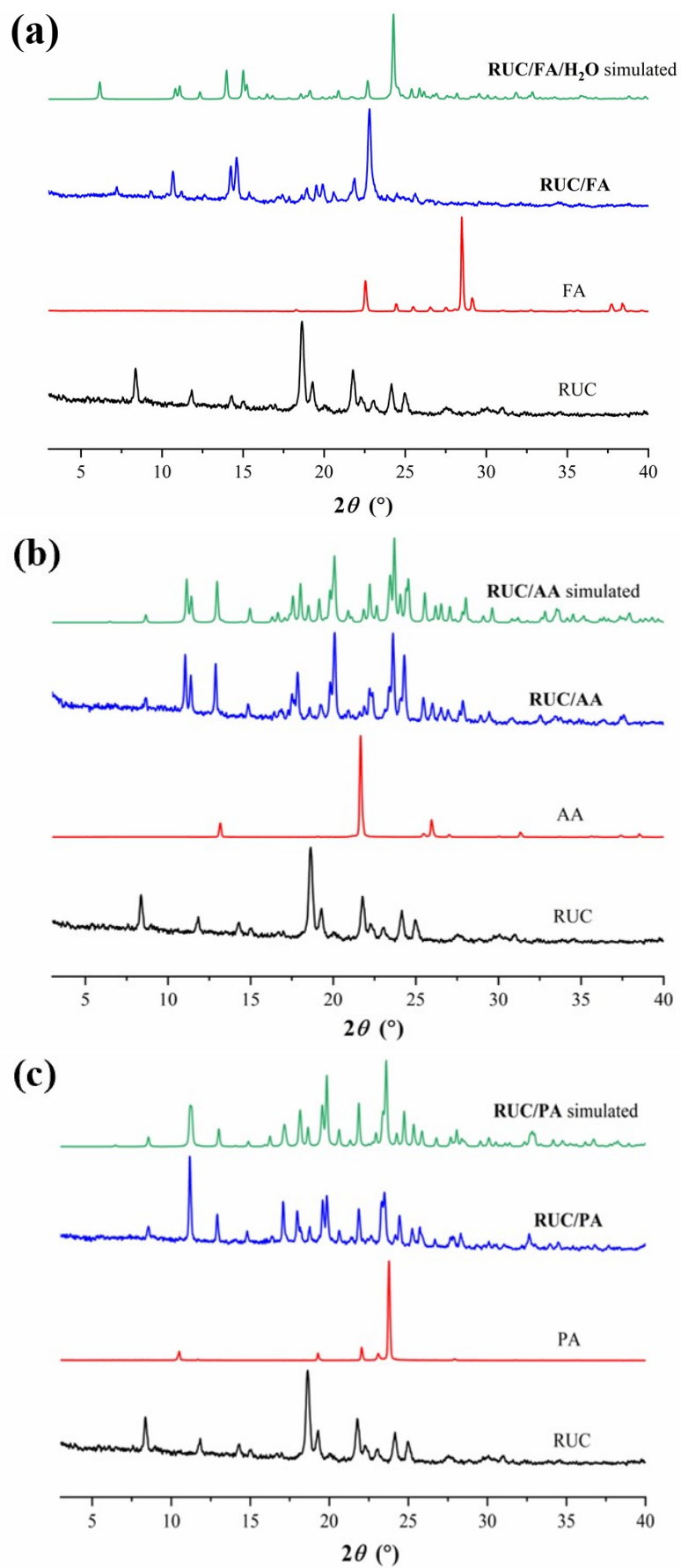
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**Table S1.** Outcome of cocrystallization screening of RUC with different CFs.

API	CFs	Experimental results
Rucaparib	Adipic acid	Salt
Rucaparib	Pimelic acid	Salt
Rucaparib	Fumaric acid	Salt
Rucaparib	Gallic acid	Physical mixture
Rucaparib	Vanillic acid	Physical mixture
Rucaparib	Urea	Physical mixture
Rucaparib	Piperazine	Physical mixture
Rucaparib	Orotic acid	Physical mixture
Rucaparib	Taurine	Physical mixture
Rucaparib	<i>L</i> -(-)-Malic acid	Physical mixture
Rucaparib	Isonicotinamide	Physical mixture
Rucaparib	Mandelic acid	Physical mixture
Rucaparib	<i>L</i> -(+)-Ascorbic acid	Physical mixture
Rucaparib	Glutaric acid	Physical mixture
Rucaparib	Malonic acid	Physical mixture
Rucaparib	Glycolic acid	Physical mixture
Rucaparib	Aspartame	Physical mixture
Rucaparib	Oxamide	Physical mixture
Rucaparib	<i>D</i> -Biotin	Physical mixture
Rucaparib	Protocatechuic acid	Physical mixture
Rucaparib	3,5-Dihydroxybenzoic acid	Physical mixture
Rucaparib	Sorbic acid	Physical mixture
Rucaparib	Citric acid	Physical mixture
Rucaparib	4-Hydroxybenzoic acid	Physical mixture
Rucaparib	Hippuric acid	Physical mixture
Rucaparib	Syringic acid	Physical mixture
Rucaparib	Allantoin	Physical mixture
Rucaparib	Meglumine	Physical mixture
Rucaparib	<i>L</i> -Aspartic acid	Physical mixture
Rucaparib	Riboflavin	Physical mixture
Rucaparib	Nicotinamide	Physical mixture
Rucaparib	Suberic acid	Physical mixture

**Table S2.** Data of powder dissolution experiments of RUC salts.

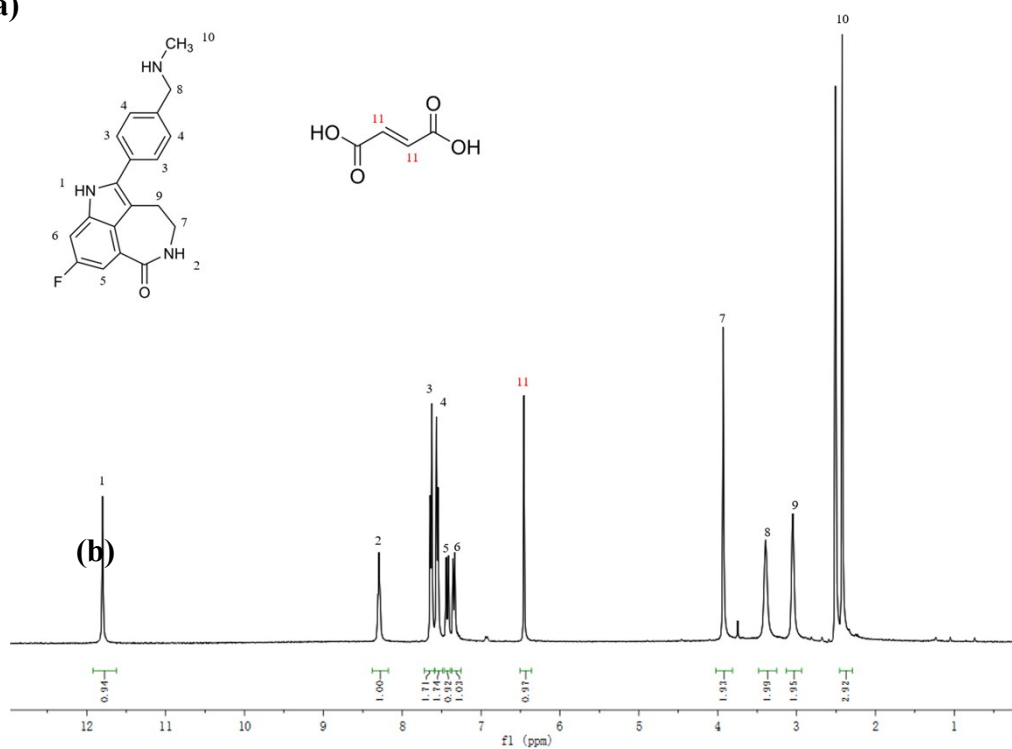
	RUC/S-CA	RUC/FA	RUC/AA	RUC/PA
$S_{\max}$ (mg/mL)	$2.9 \pm 0.2$	$2.0 \pm 0.1$	$4.2 \pm 0.2$	$4.7 \pm 0.1$
fold	1	0.69	1.4	1.6



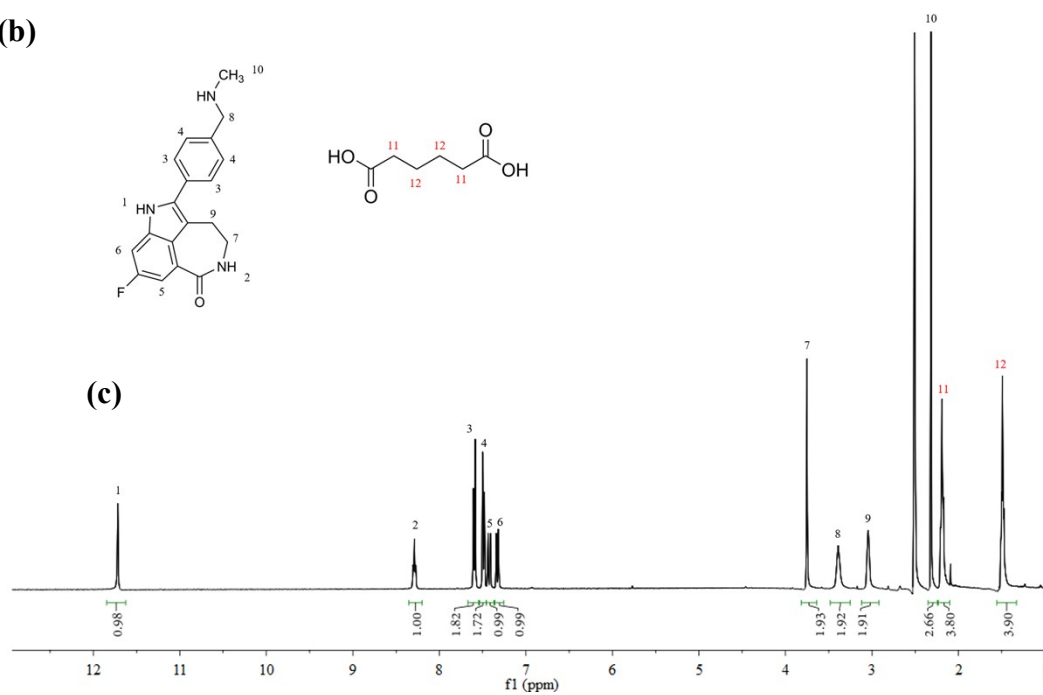
**Fig. S1** PXRd patterns of RUC, FA/AA/PA and the synthesized salts, and simulated from SXRD data for (a) RUC/FA, (b) RUC/AA and (c) RUC/PA.

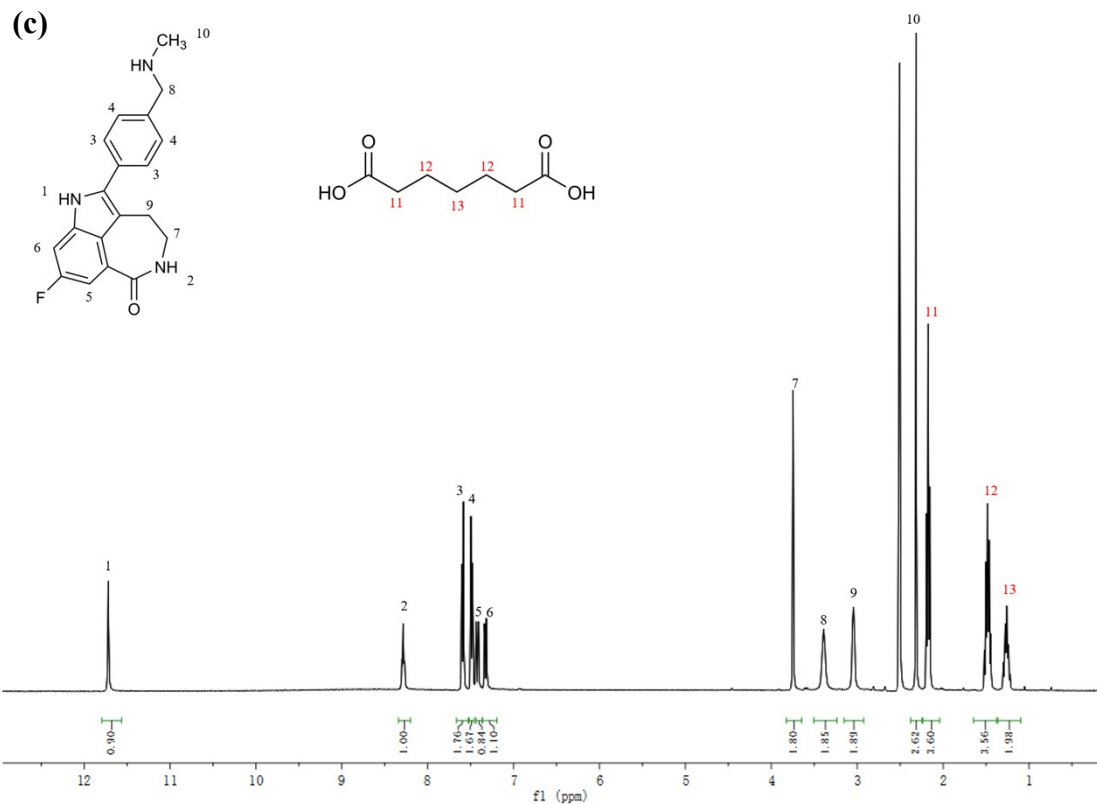
Fig. S2 TG-DSC curves of (a) RUC/FA, (b) RUC/AA and (c) RUC/PA.

(a)

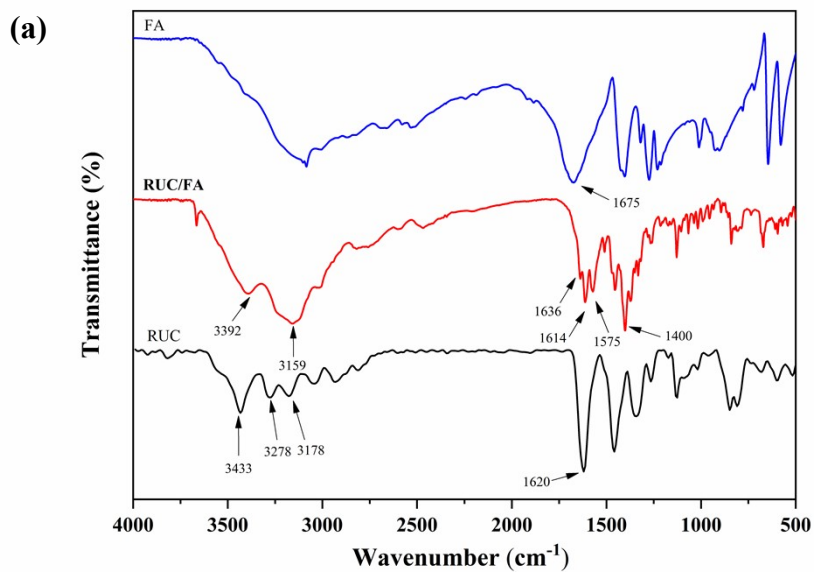


(b)

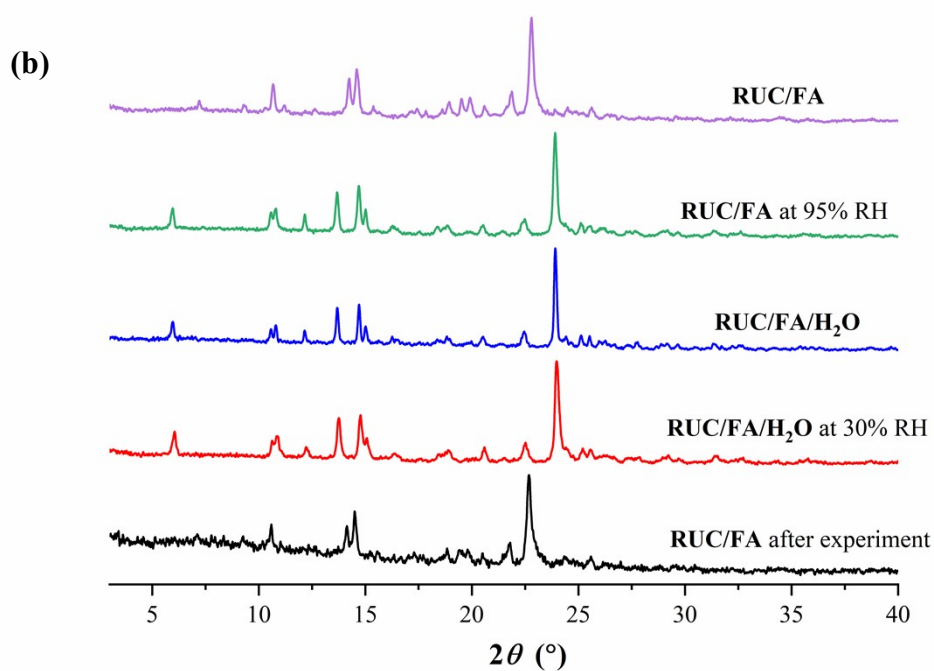
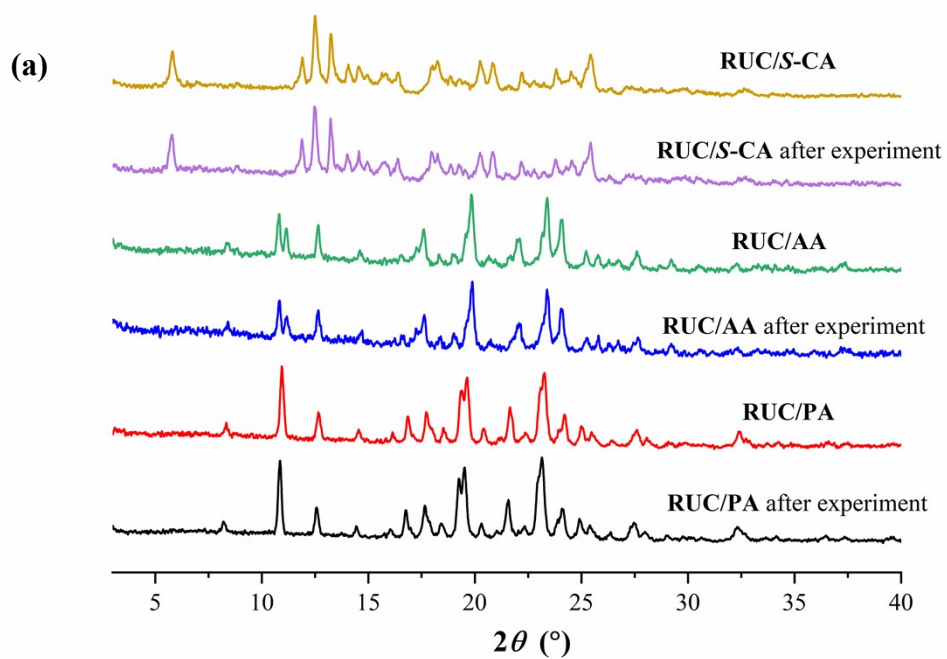




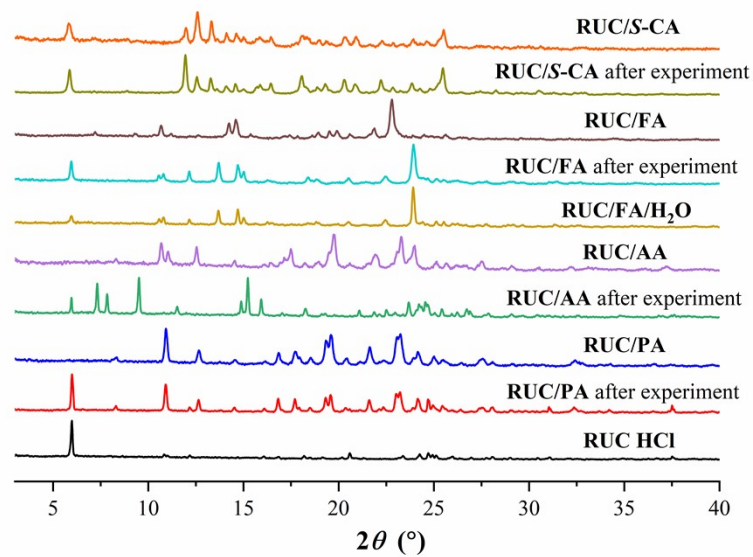
**Fig. S3**  $^1\text{H}$  NMR spectra of (a) RUC/FA, (b) RUC/AA and (c) RUC/PA.



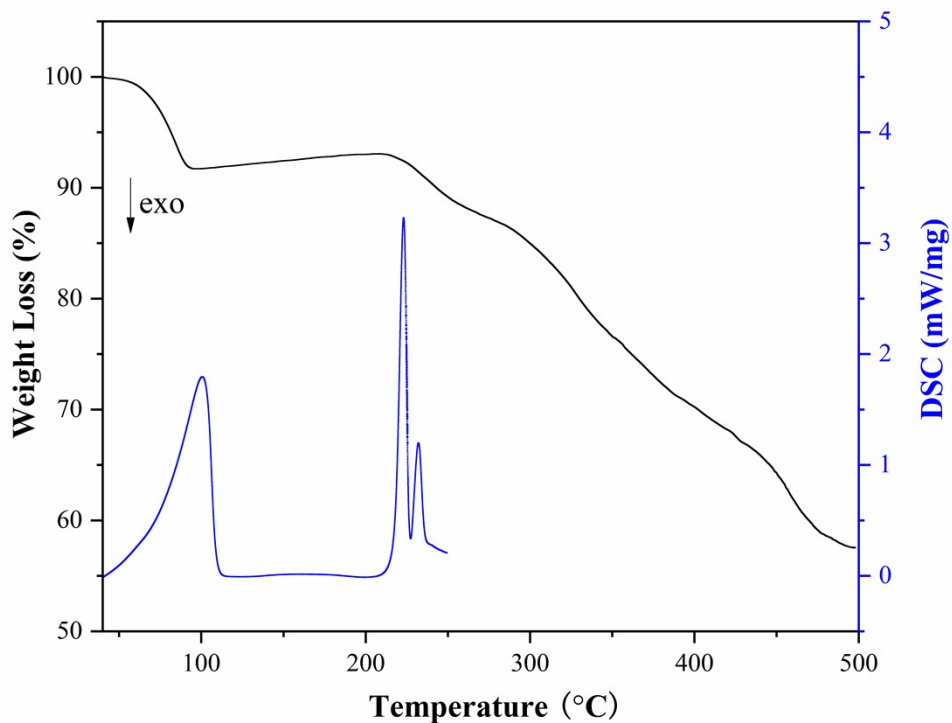
**Fig. S4** FT-IR spectra of (a) RUC/FA, (b) RUC/AA and (c) RUC/PA.



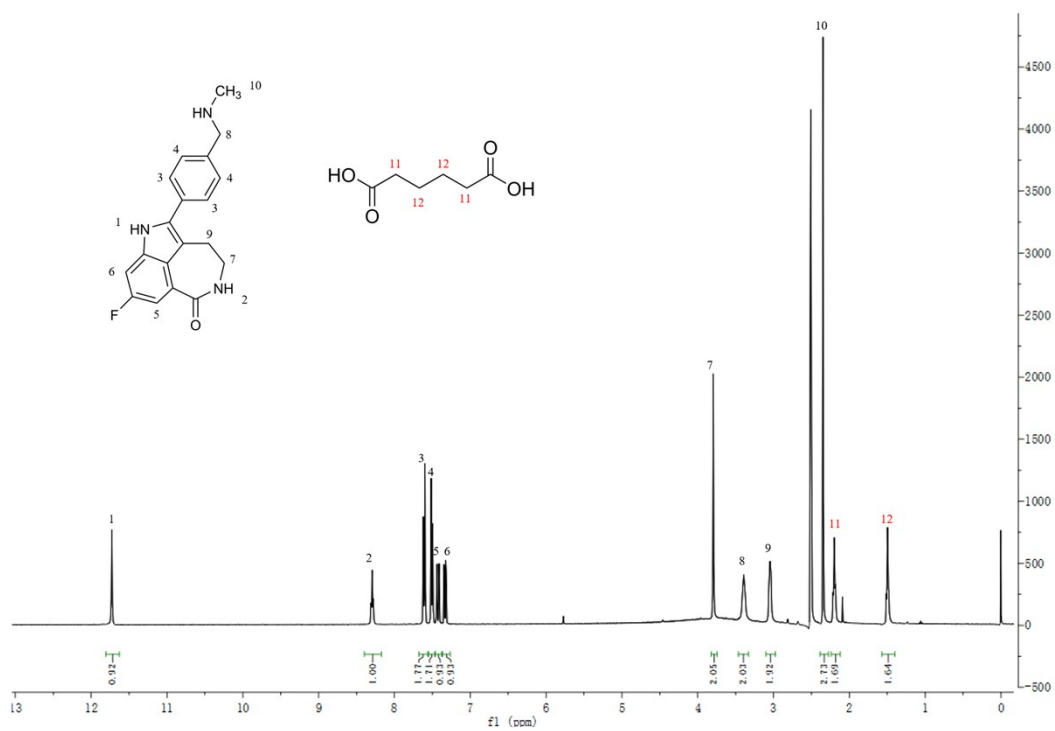
**Fig. S5** PXR D patterns of (a) RUC/S-CA, RUC/AA and RUC/PA and (b) RUC/FA before and after DVS tests.



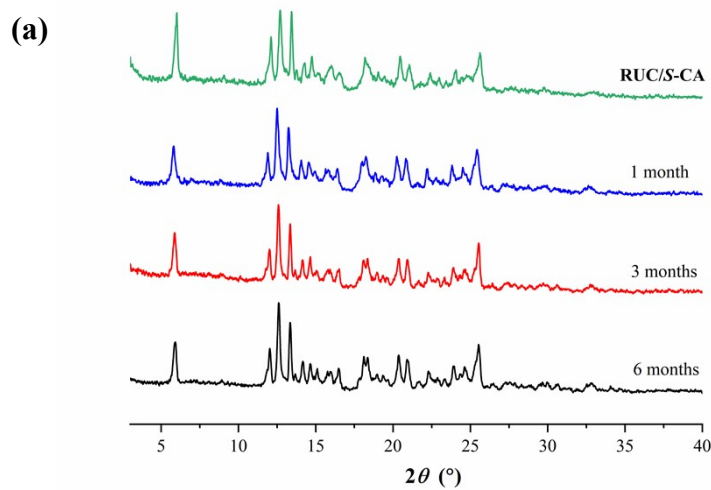
**Fig. S6** PXRD patterns of residual solids after powder dissolution experiments for **RUC/S-CA**, **RUC/FA**, **RUC/AA** and **RUC/PA**.



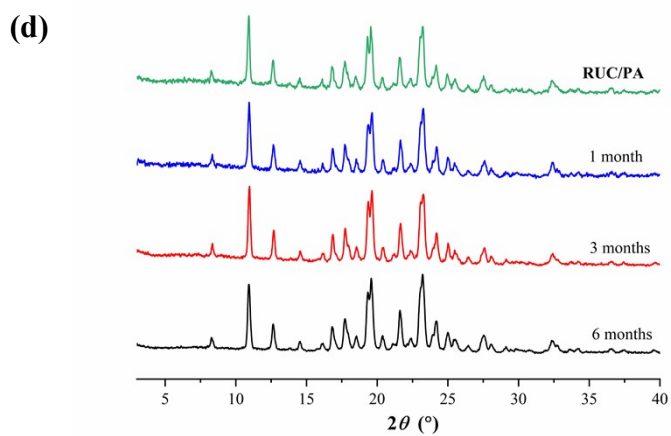
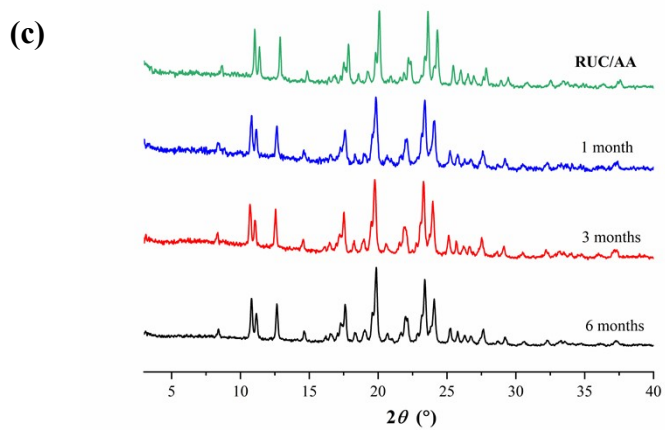
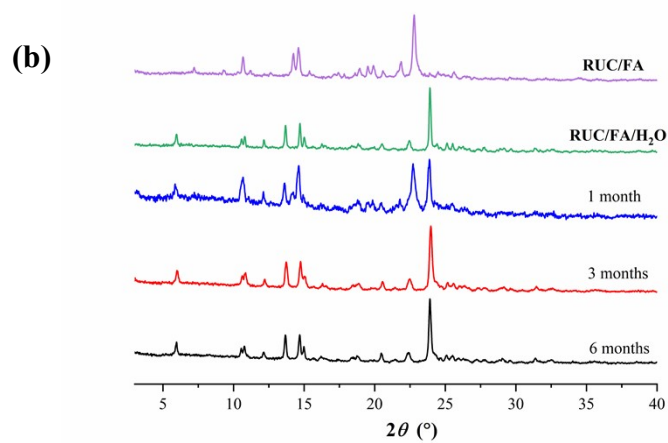
**Fig. S7** TG-DSC curves for **RUC/AA/H<sub>2</sub>O**.



**Fig. S8**  $^1\text{H}$  NMR spectra of RUC/AA/H<sub>2</sub>O.







**Fig. S9** PXRd patterns of (a) RUC/S-CA, (b) RUC/FA, (c) RUC/AA and (d) RUC/PA after accelerated stability tests.