

Supplementary Materials

Table S1. Comparison of the 2 θ angle data of the Febuxostat (FB)-L-pyroglutamic acid (PG) cocrystal and FB polymorphs.

PXRD Angle 2-Theta °					
FB-PG	Form A	Form B	Form C	Form D	Form G
6.90	6.62	6.76	6.62	8.32	6.86
7.42	7.18	8.08	10.80	9.68	8.36
8.45	12.80	9.74	13.36	12.90	9.60
9.94	13.26	11.50	15.50	16.06	11.76
10.26	16.48	12.20	16.74	17.34	13.74
10.62	19.58	13.56	17.40	19.38	14.60
13.29	21.92	15.76	18.00	21.56	15.94
13.57	22.68	16.20	18.70	24.06	16.74
14.52	25.84	17.32	20.16	26.00	17.56
16.06	26.70	19.38	20.62	30.06	20.00
16.66	29.20	21.14	24.78	33.60	21.26
18.84	36.70	21.56	25.18	40.34	23.72
19.14		25.72	34.08		24.78
19.97		27.68	36.72		25.14
20.54		29.36	38.04		25.74
21.34					26.64
21.79					27.92
23.63					
24.10					
24.74					
26.90					

Table S2. Comparison of the 2 θ angle data of the FB-PG cocrystal, FB, and P.G

PXRD Angle 2-Theta °		
FB-PG	FB Form A	PG
6.90	6.62	11.524
7.42	7.18	12.151
8.45	12.80	12.719
9.94	13.26	13.223
10.26	16.48	14.095
10.62	19.58	14.483
13.29	21.92	15.185
13.57	22.68	15.629
14.52	25.84	16.982
16.06	26.70	17.51
16.66	29.20	19.109
18.84	36.70	19.673
19.14		20.649
19.97		21.325
20.54		21.525
21.34		21.777
21.79		22.197
23.63		23.074
24.10		23.823
24.74		
26.90		

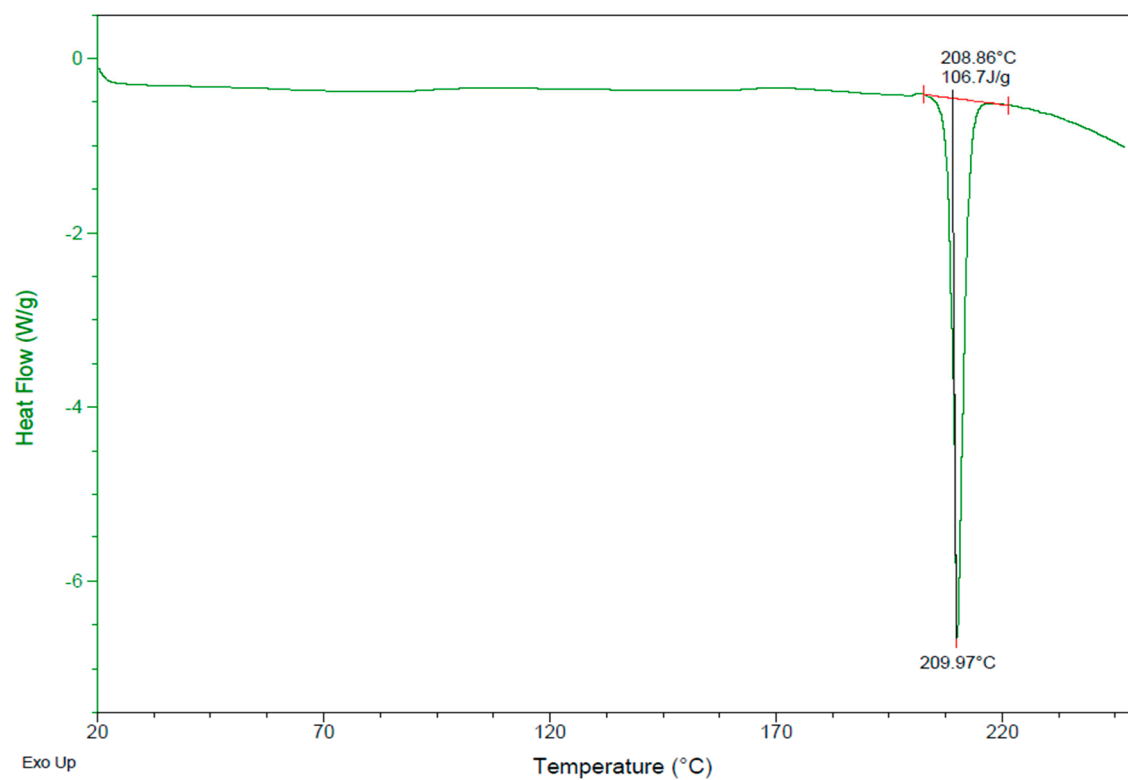


Figure S1. Differential scanning calorimetry (DSC) curve of FB form-A (heating rate 10 °C/min).

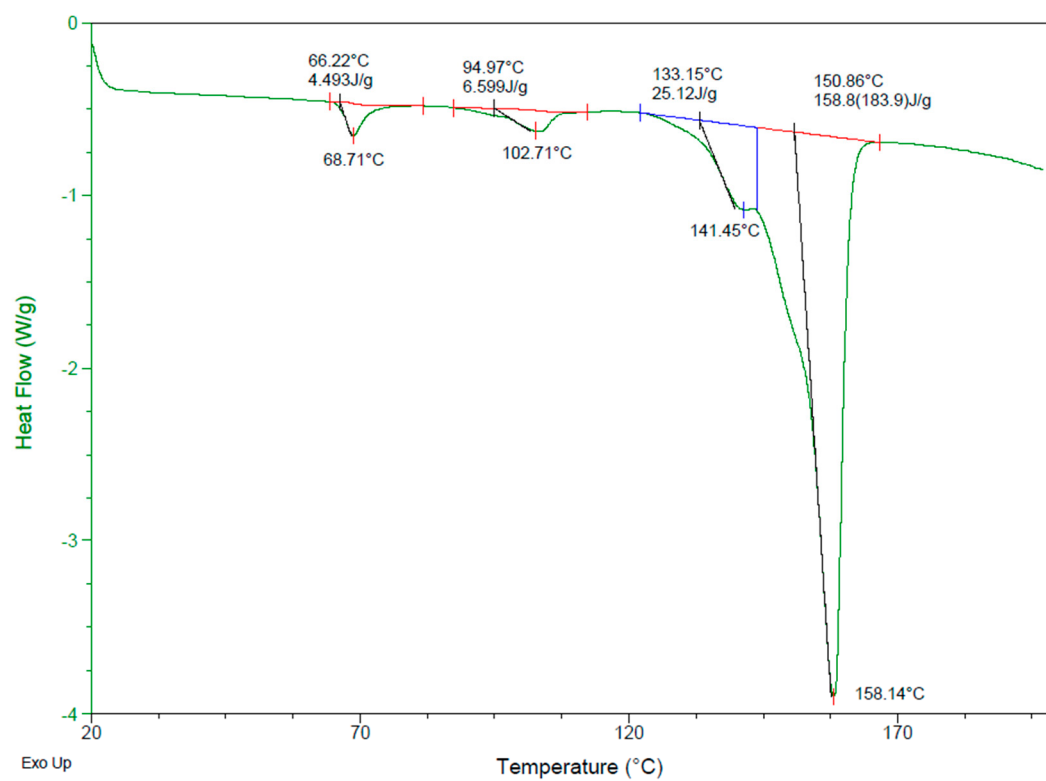


Figure S2. DSC curve of PG (heating rate 10 °C/min).

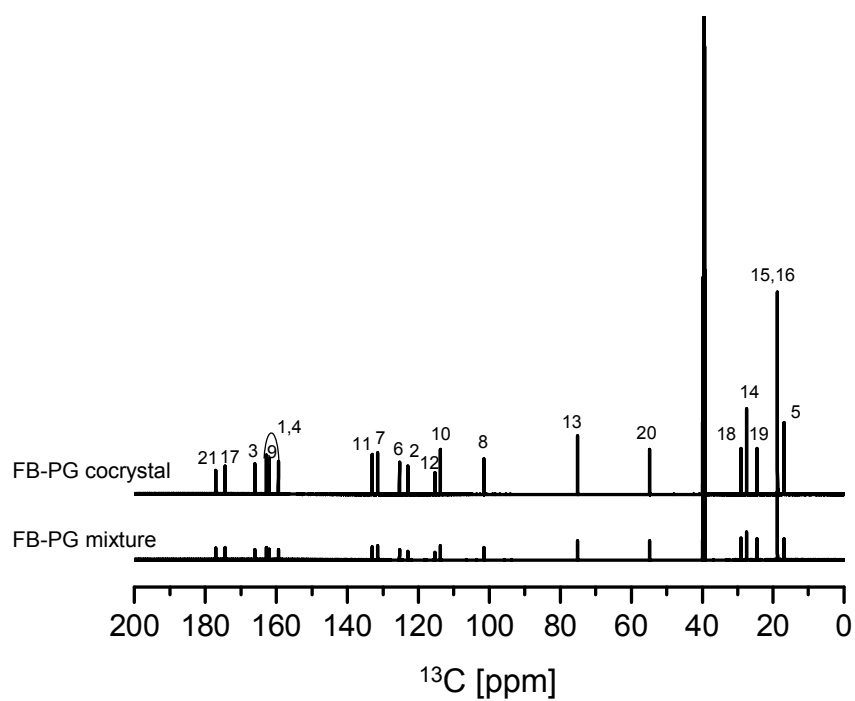


Figure S3. Solution-state ^{13}C -NMR data of FB/PG (2:1) mixture and FB-PG cocrystal ($\text{DMSO-}d_6$).

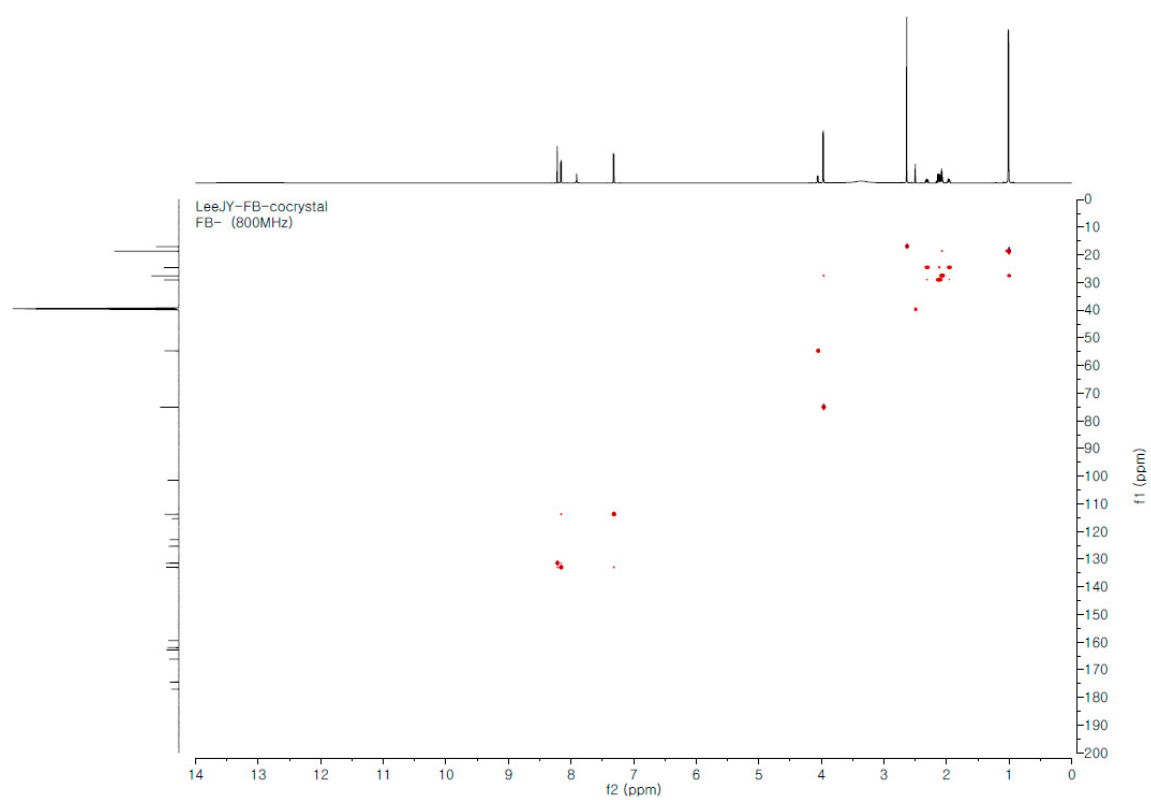


Figure S4. Solution-state 2D (^1H - ^{13}C HSQC) NMR data of FB-PG cocrystal ($\text{DMSO}-d_6$).

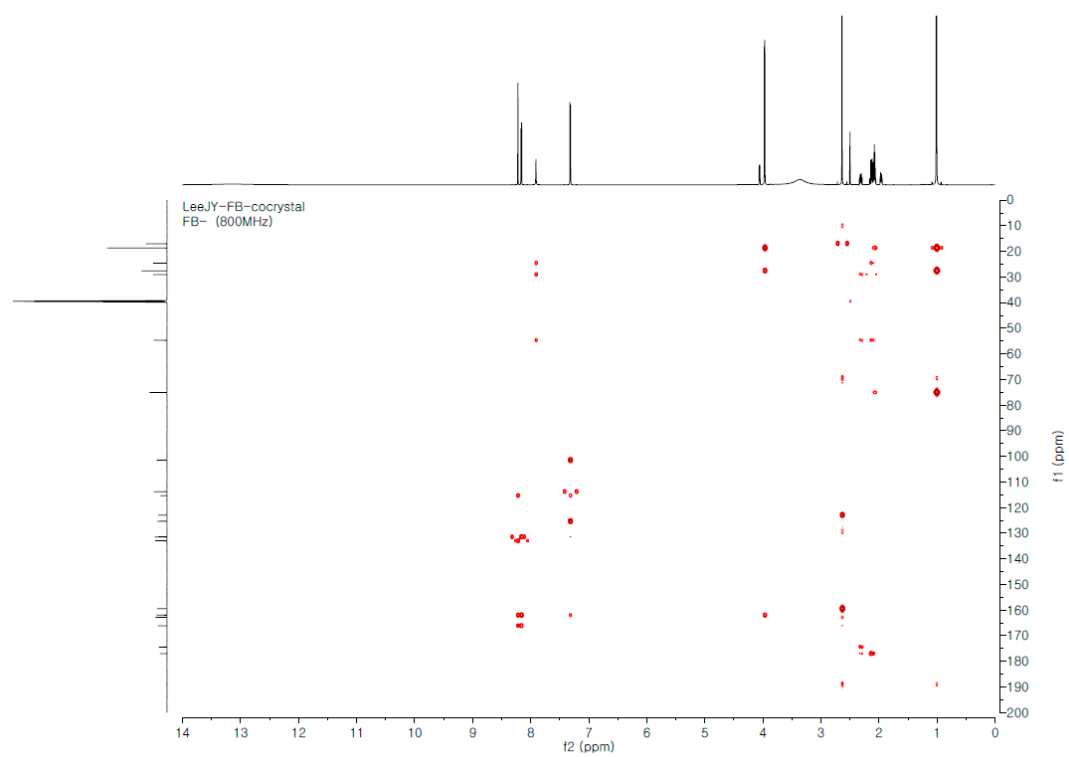


Figure S5. Solution-state 2D (^1H - ^{13}C HMBC) NMR data of FB-PG cocrystal ($\text{DMSO}-d_6$).

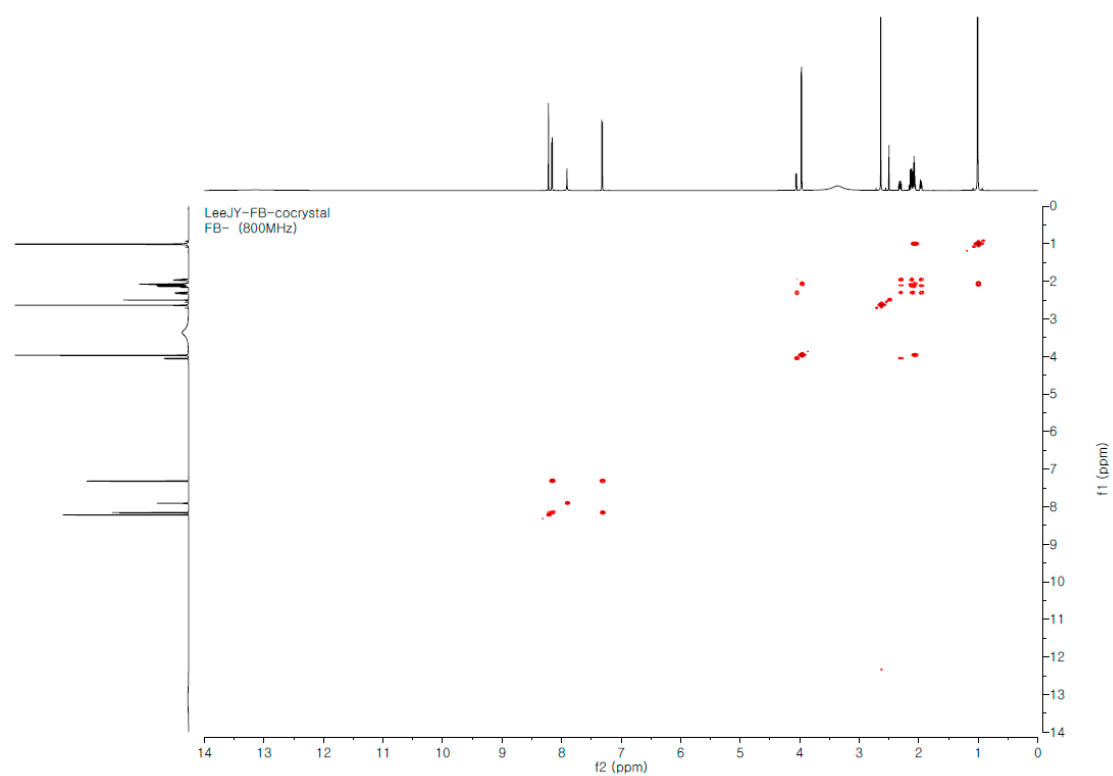


Figure S6. Solution-state 2D (^1H - ^1H COSY) NMR data of FB-PG cocrystal ($\text{DMSO-}d_6$).

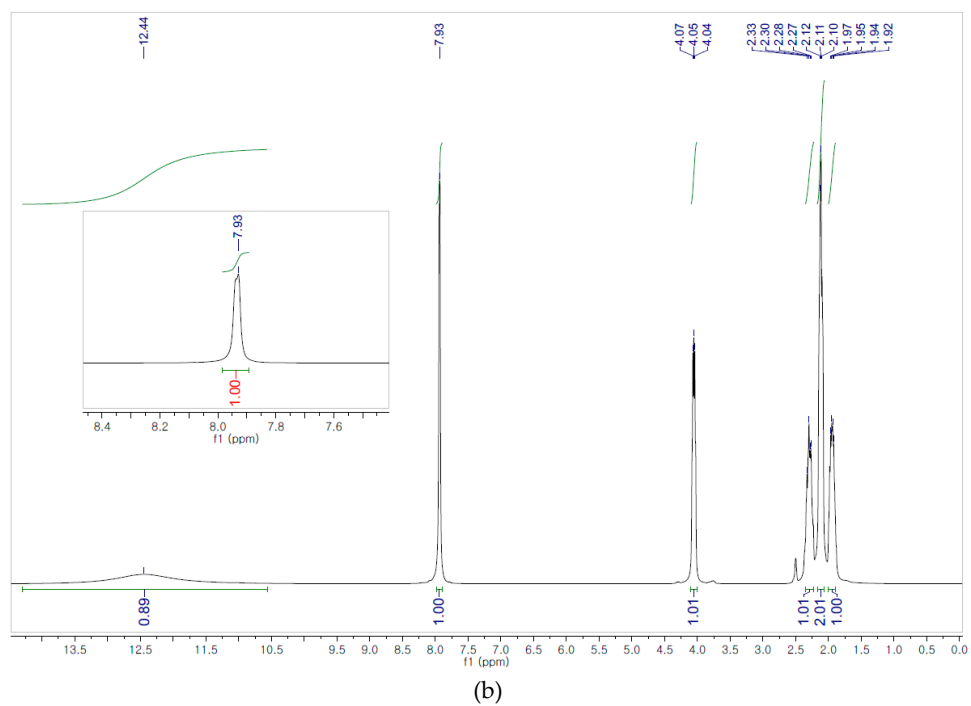
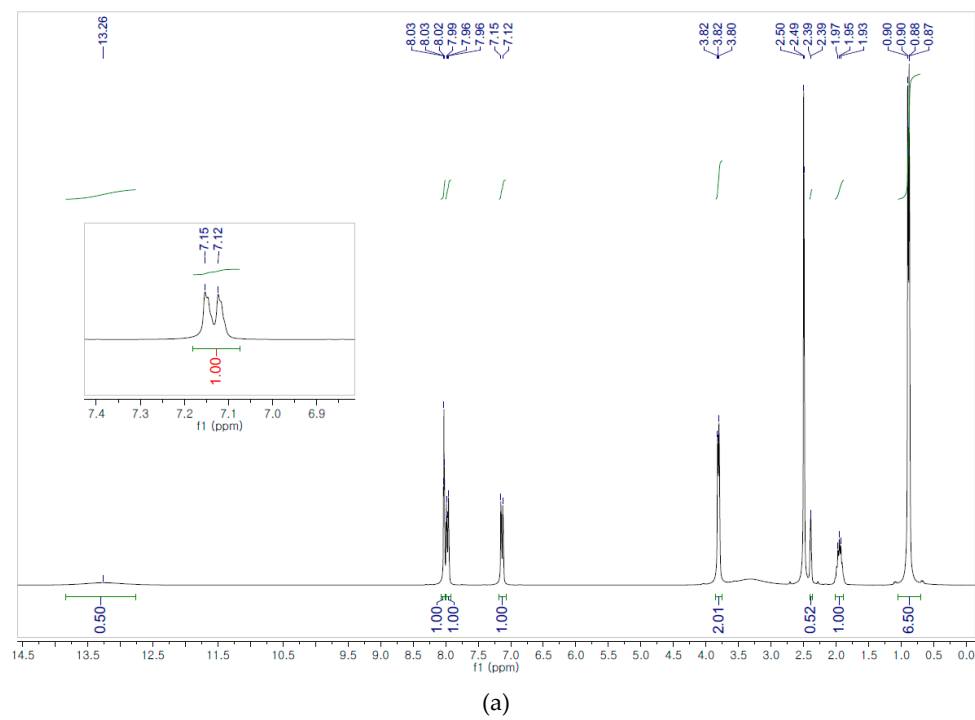


Figure S7. Solution-state ^1H -NMR data of FB and PG ($\text{DMSO}-d_6$): (a) FB, (b) PG ($\text{DMSO}-d_6$).