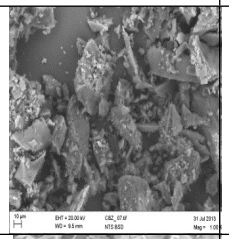
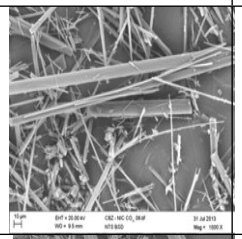
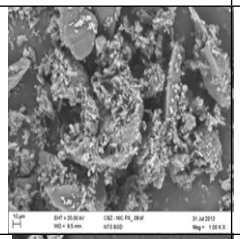
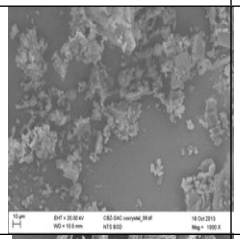
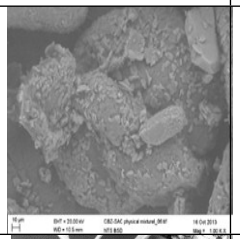
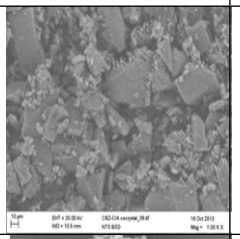
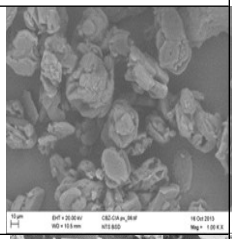
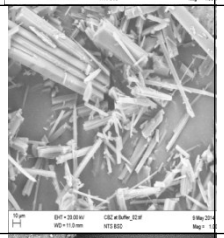
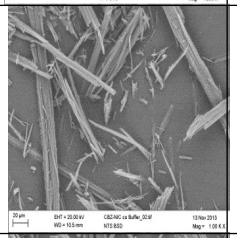
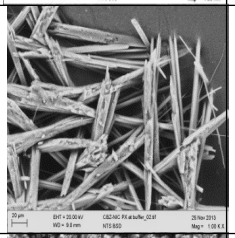
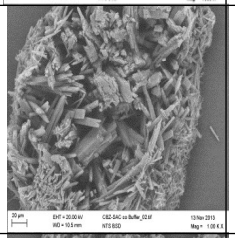
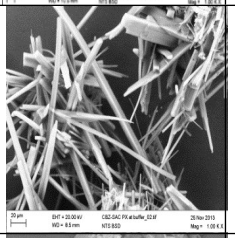
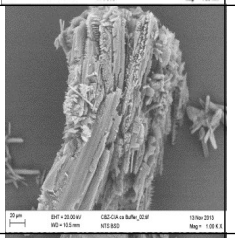
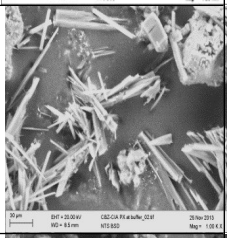
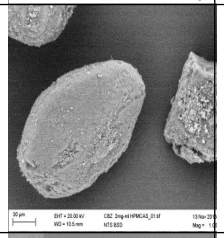
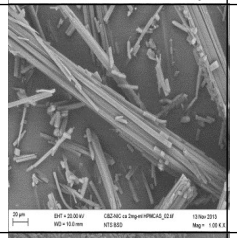
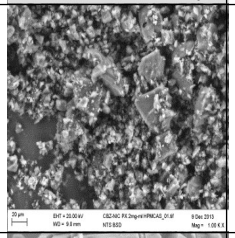
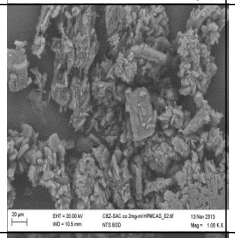
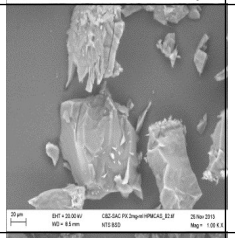
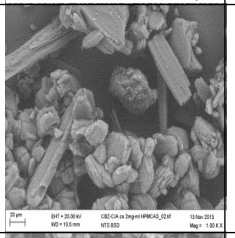
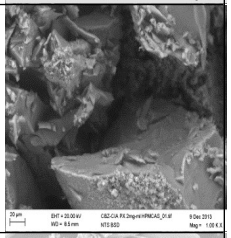
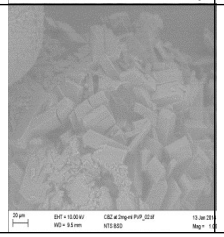
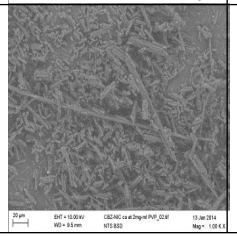
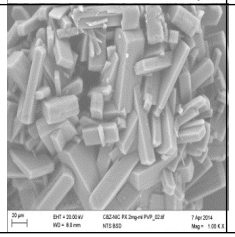
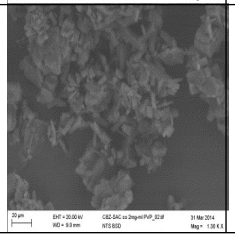
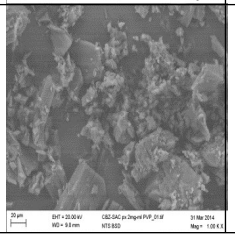
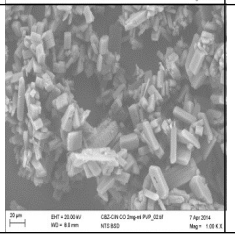
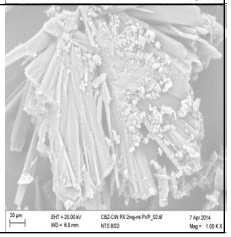
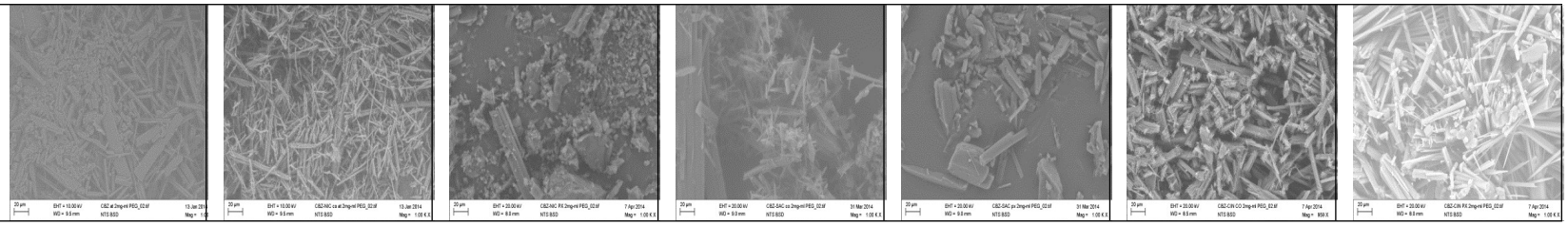
Electronic Supplementary Material (ESI) for CrystEngComm.

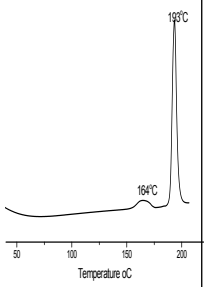
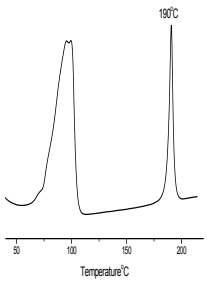
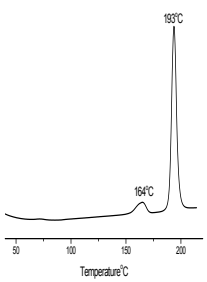
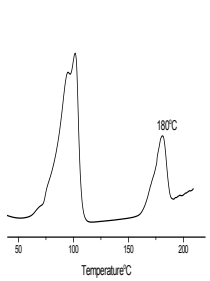
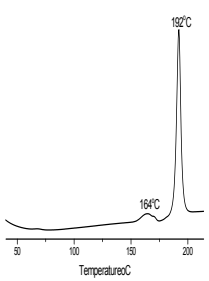
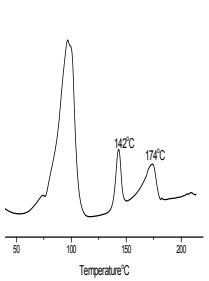
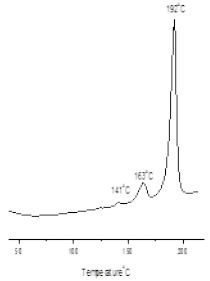
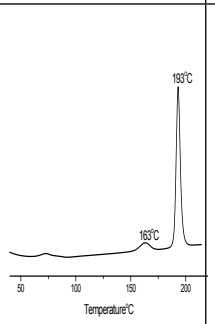
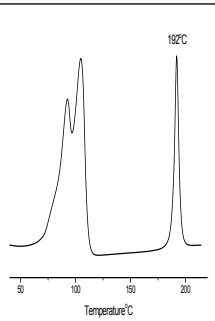
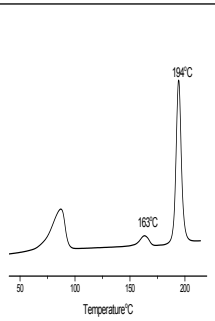
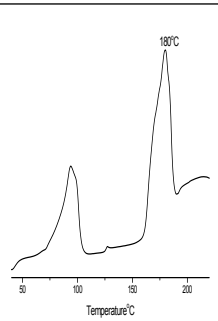
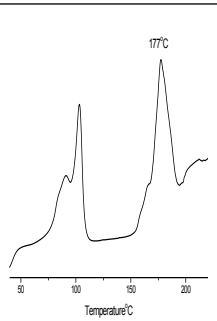
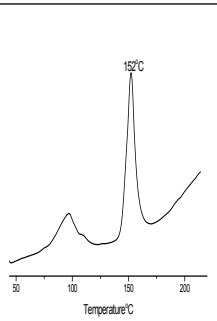
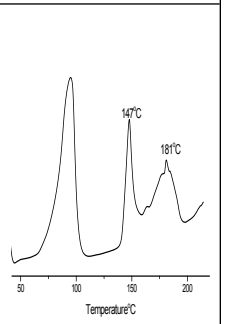
Fig. S1 SEM photographs of original samples and solid residues retrieved from solubility studies in the absence and presence of 2 mg/ml polymer in pH6.8 PBS

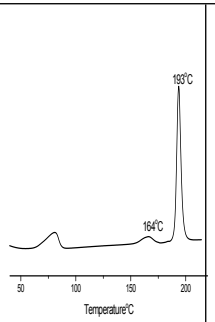
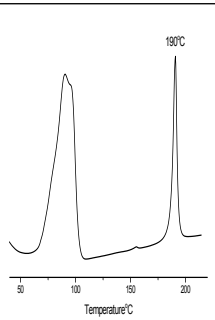
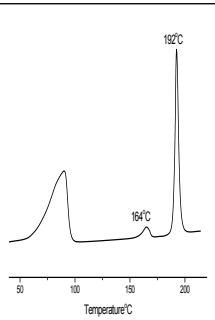
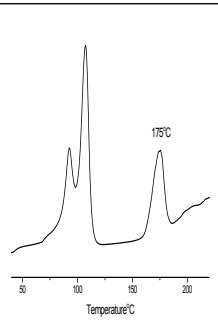
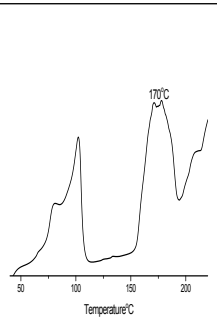
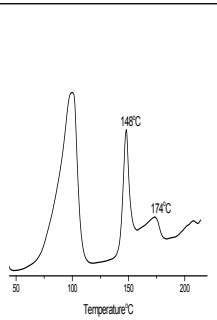
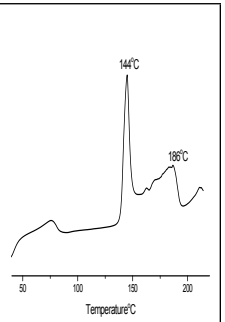
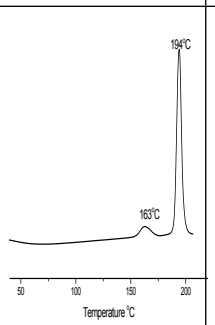
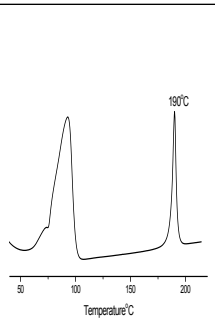
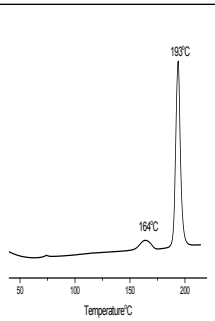
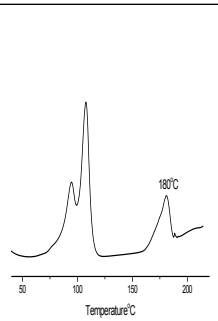
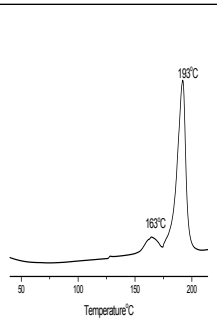
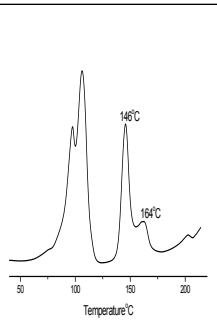
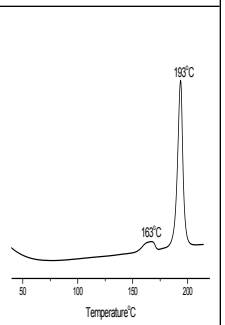
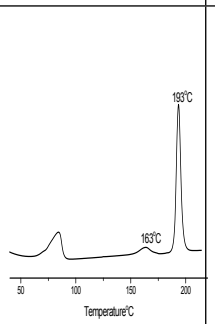
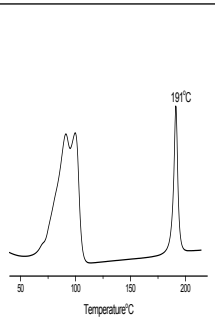
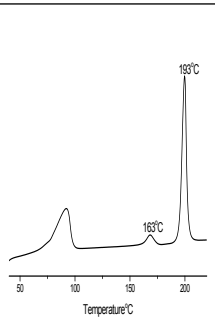
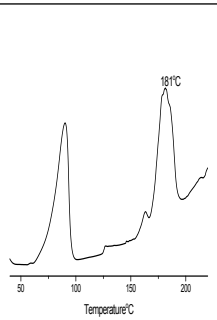
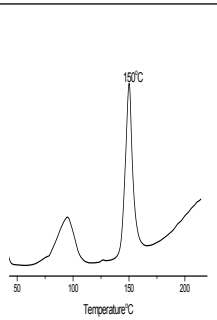
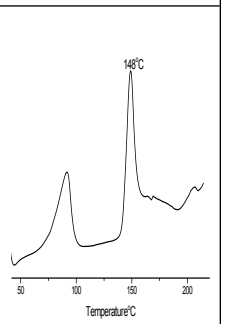
		CBZ III	CBZ-NIC cocrystal	CBZ-NIC mixture	CBZ-SAC cocrystal	CBZ-SAC mixture	CBZ-CIN cocrystal	CBZ-CIN mixture
Original								
pH 6.8 PBS								
pH 6.8 PBS in the presence of 2mg/ml	HPMCAS							
	PVP							

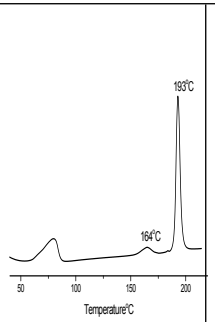
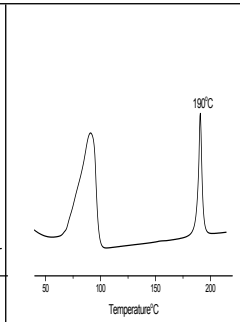
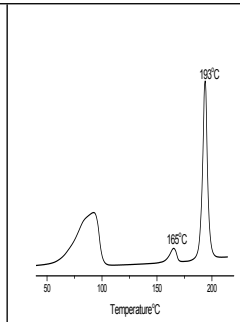
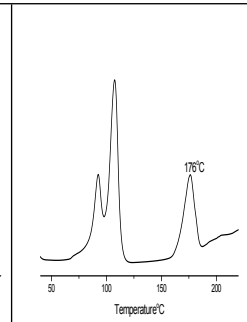
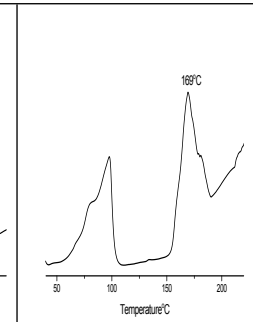
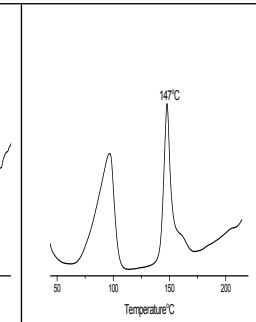
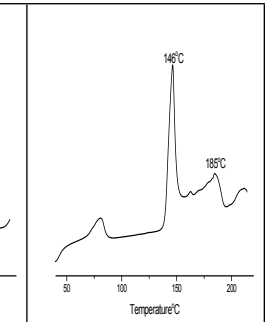
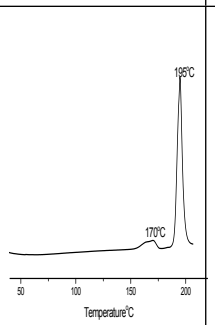
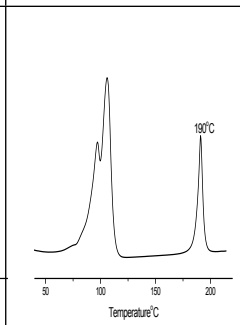
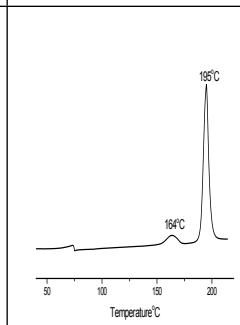
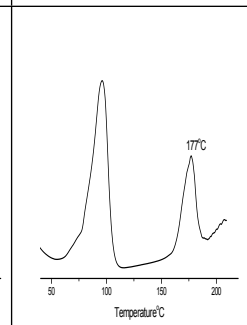
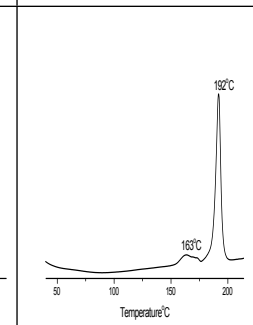
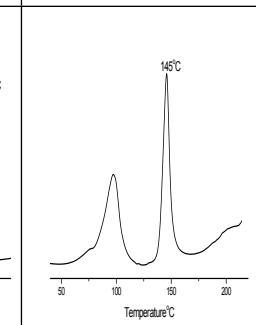
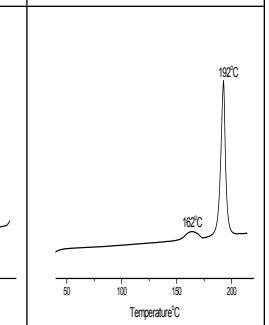
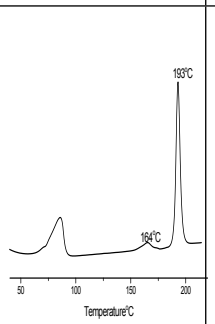
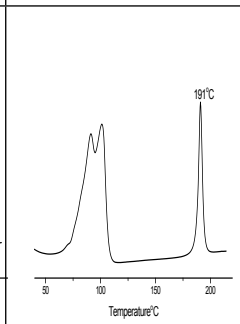
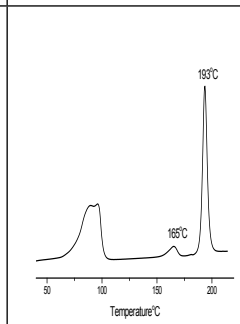
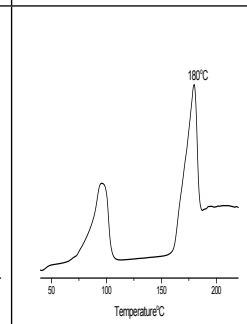
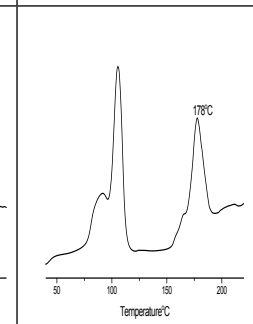
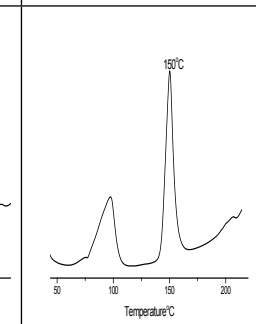
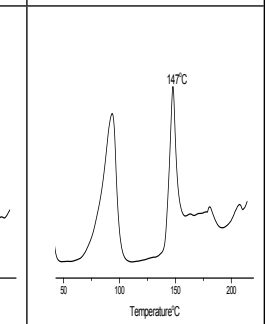
	PEG	

Note: The original CBZ III samples appeared to be irregular which were mixtures of prismatic and rock shape particles and they became CBZ DH crystals showing needle-like shape after the test in the absence of a polymer. The solid residues in the presence of 2 mg/mL HPMCAS in pH6.8 PBS had the similar shape as those of the original CBZ III, indicating that there was no phase transformation. In the solid residues of the test in the presence of 2 mg/mL PVP or PEG, it was a mixture of needle-like (CBZ DH) and prismatic/rock (CBZ III) particles.

Figure S2. DSC thermographs of solid residues retrieved from solubility studies in the presence of different concentrations of a polymer in pH6.8 PBS

Polymer (mg/ml)		CBZ III	CBZ-NIC cocrystal	CBZ-NIC mixture	CBZ-SAC cocrystal	CBZ-SAC mixture	CBZ-CIN cocrystal	CBZ-CIN mixture
0.5	HPMC AS							
	PVP							

	PEG							
1.0	HPMC AS							
	PVP							

	PEG							
5.0	HPMC AS							
	PVP							

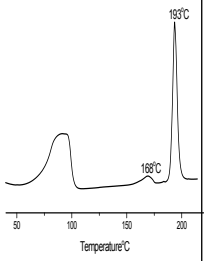
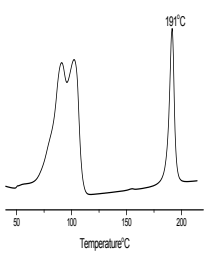
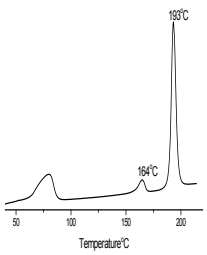
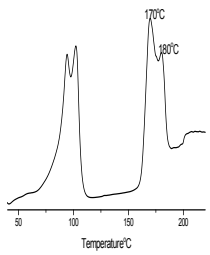
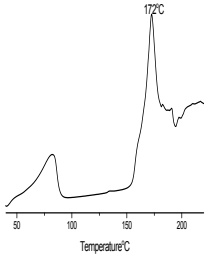
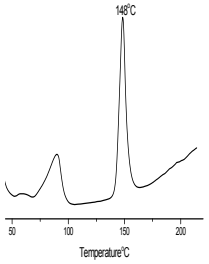
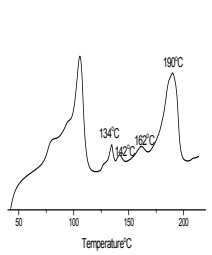
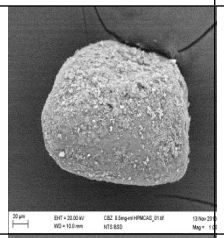
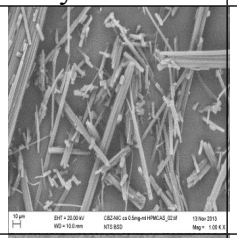
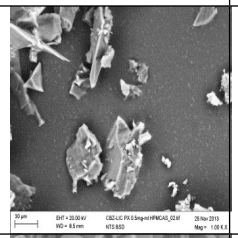
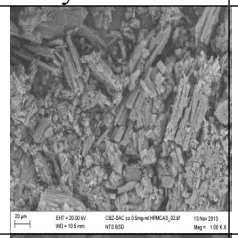
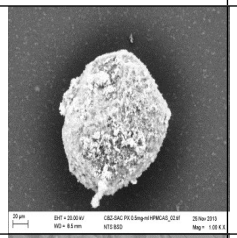
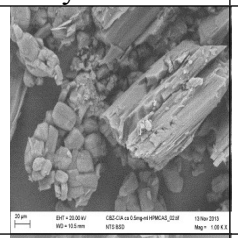
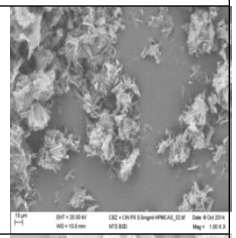
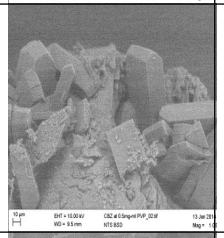
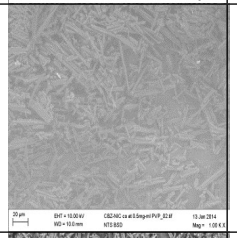
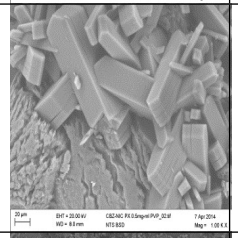
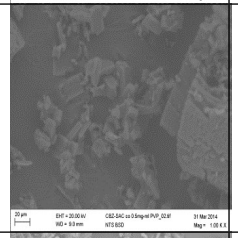
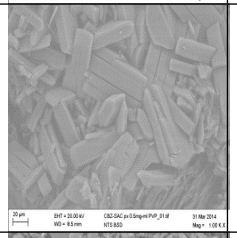
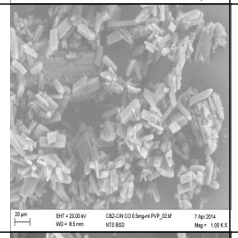
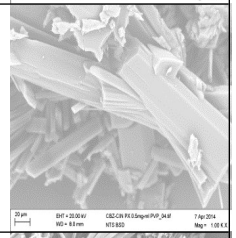
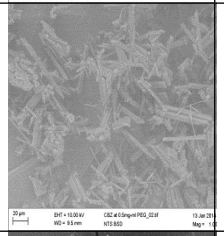
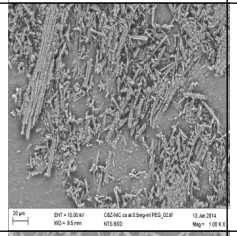
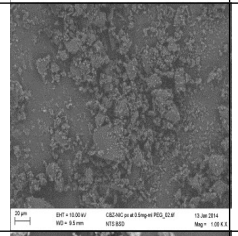
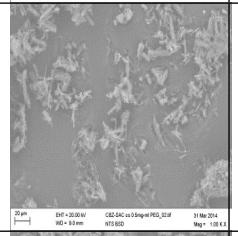
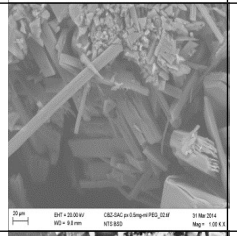
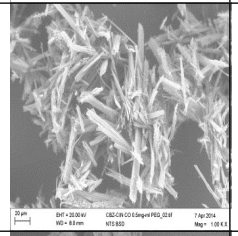
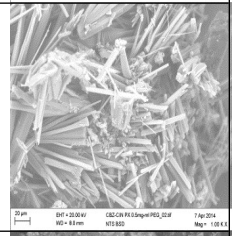
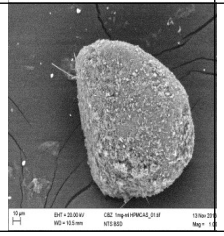
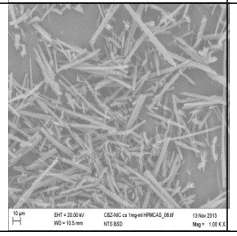
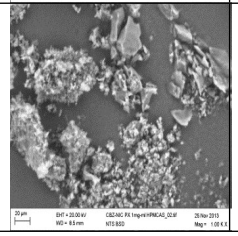
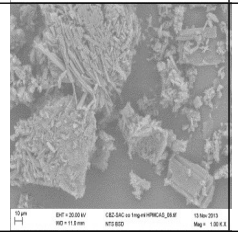
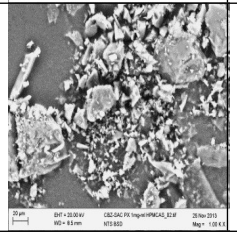
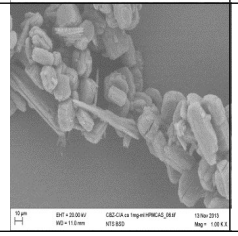
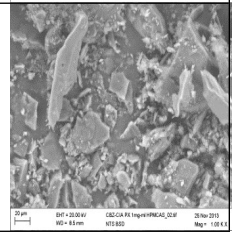
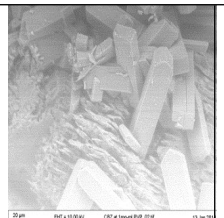
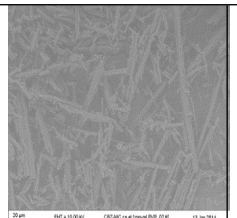
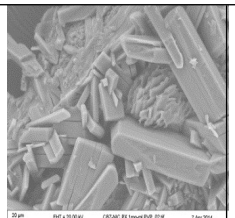
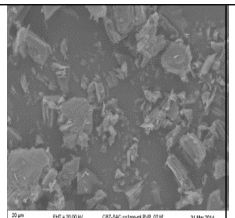
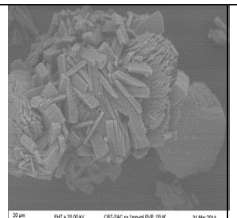
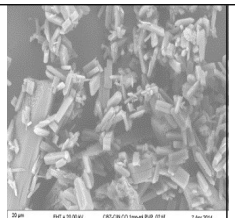
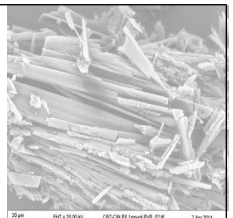
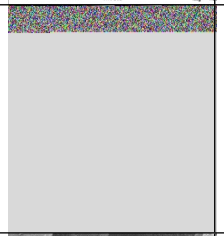
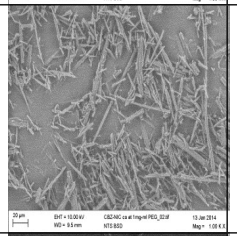
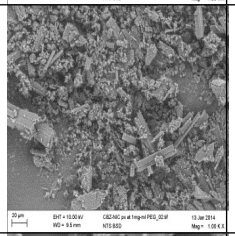
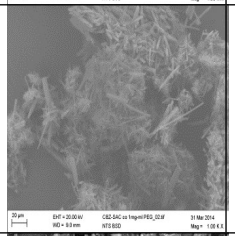
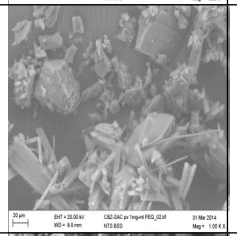
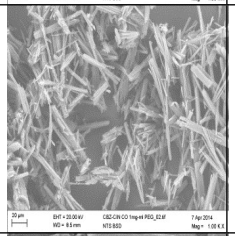
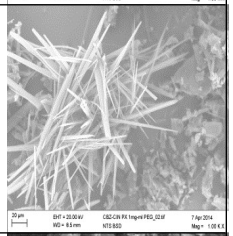
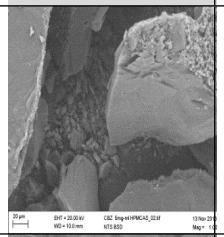
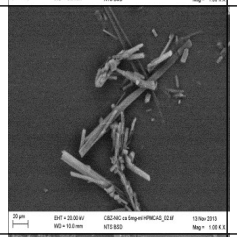
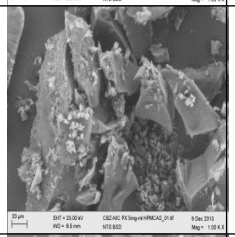
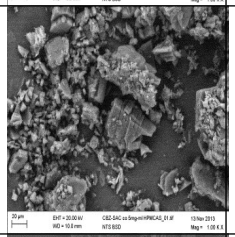
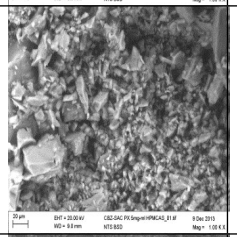
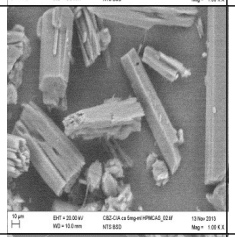
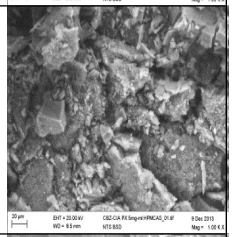
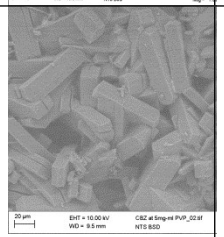
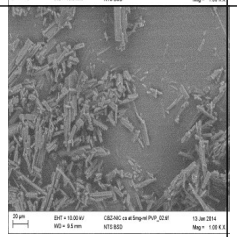
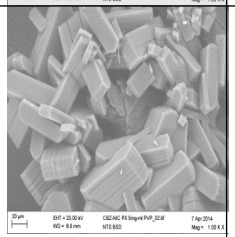
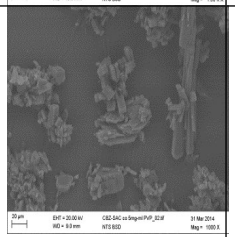
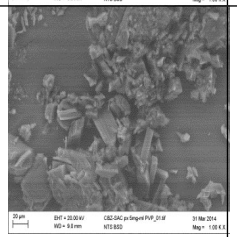
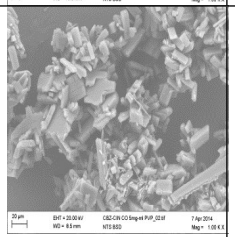
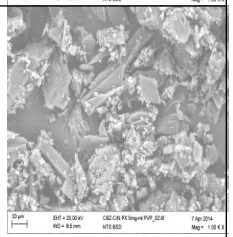
	PEG	 193°C 168°C 50 100 150 200 Temperature°C	 191°C 50 100 150 200 Temperature°C	 193°C 164°C 50 100 150 200 Temperature°C	 170°C 180°C 50 100 150 200 Temperature°C	 172°C 50 100 150 200 Temperature°C	 148°C 50 100 150 200 Temperature°C	 190°C 134°C 142°C 162°C 50 100 150 200 Temperature°C

Figure S3. SEM photographs of the solid residues retrieved from solubility studies in the presence of different concentrations of a polymer in pH6.8 PBS

Polymer (mg/ml)		CBZ III	CBZ-NIC cocrystal	CBZ-NIC mixture	CBZ-SAC cocrystal	CBZ-SAC mixture	CBZ-CIN cocrystal	CBZ-CIN mixture
0.5	HPMC AS							
	PVP							
	PEG							
1.0	HPMC AS							

	PVP								
	PEG								
5.0	HPMC AS								
	PVP								

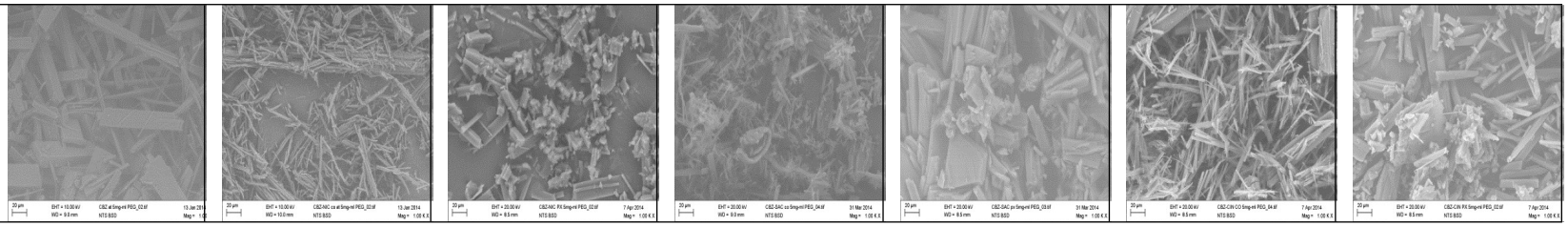
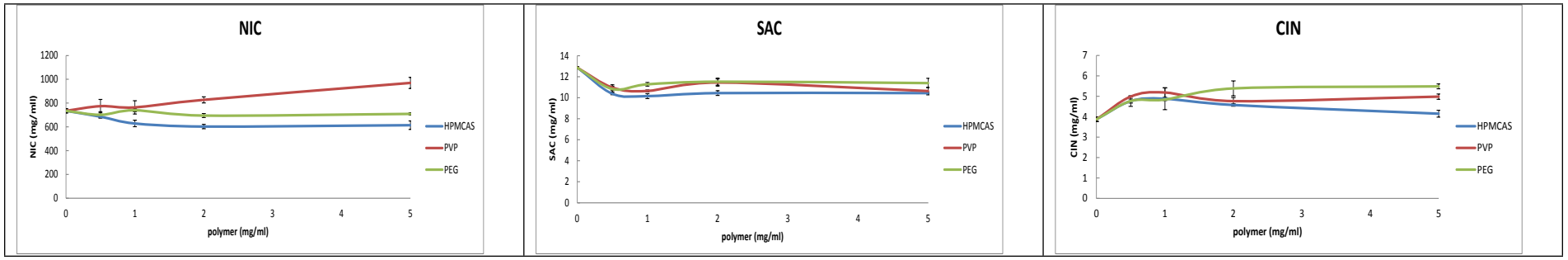
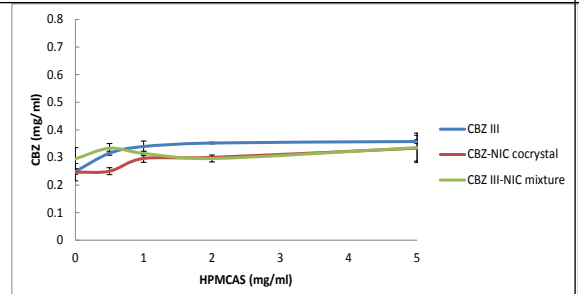
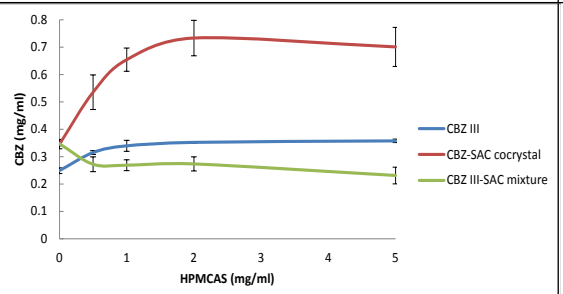
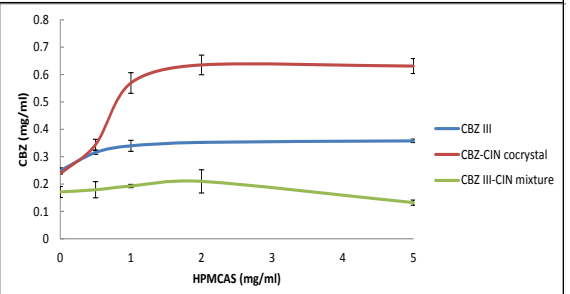
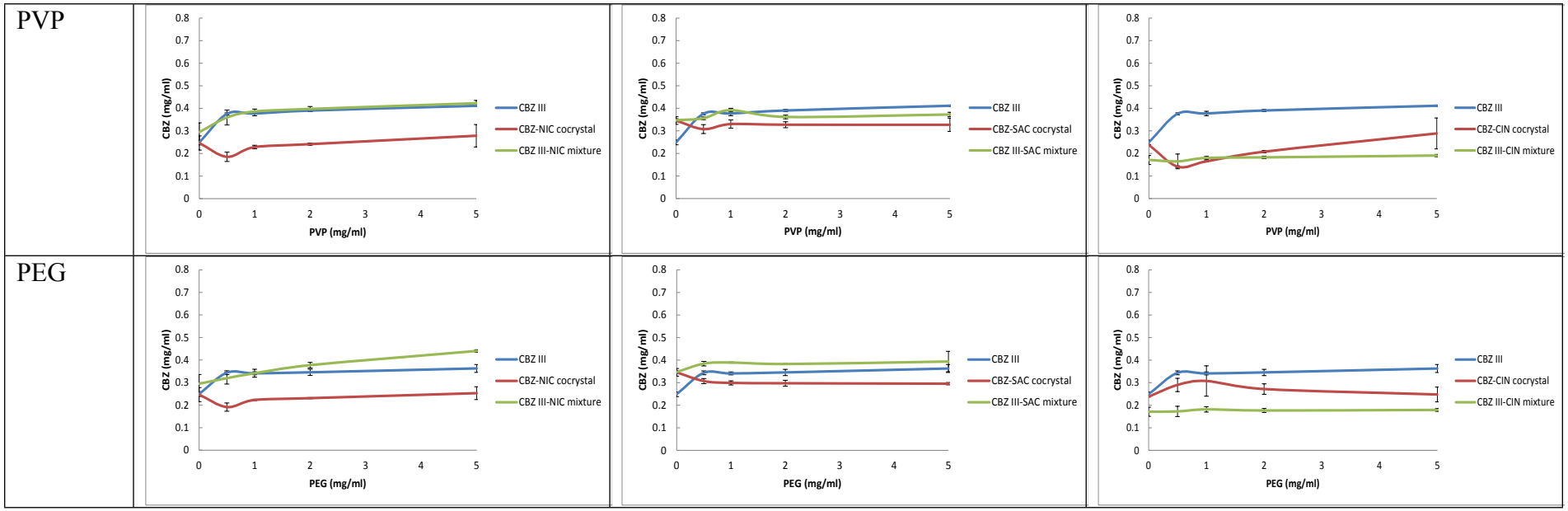
	PEG	

Figure S4. Coformer concentrations and comparison of CBZ concentrations of CBZ III, CBZ cocrytals and physical mixtures in the absence and presence of the different concentrations of pre-dissolved polymers in pH6.8 PBS at equilibrium after 24 h: (a) coformer concentration; (b) comparisons of CBZ concentrations of CBZ III, CBZ cocrytals and physical mixtures



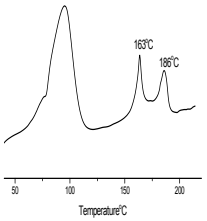
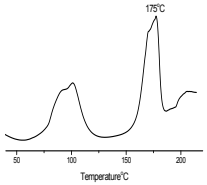
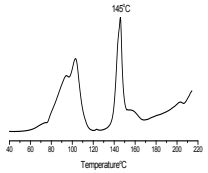
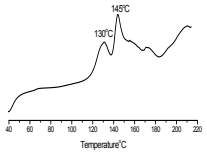
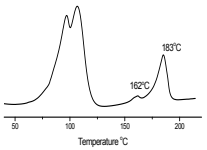
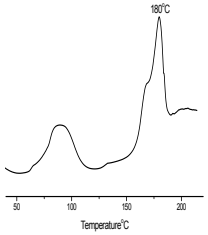
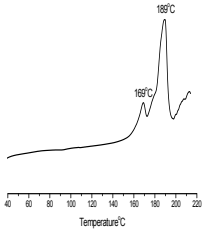
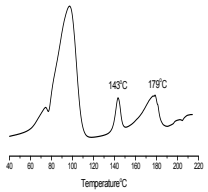
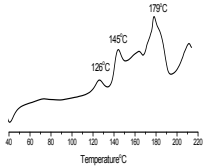
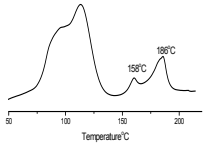
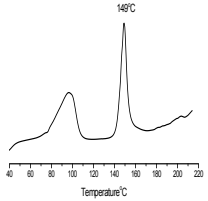
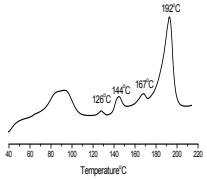
`(a)

	CBZ concentrations of CBZ III, CBZ-NIC cocrystal and physical mixture of CBZ III-NIC	CBZ concentrations of CBZ III, CBZ-SAC cocrystal and physical mixture of CBZ III-SAC	CBZ concentrations of CBZ III, CBZ-CIN cocrystal and physical mixture of CBZ III-CIN
HPMCAS			


PVP
PEG
CBZ (mg/ml)
PVP (mg/ml)
PEG (mg/ml)
CBZ III
CBZ-NIC cocrystal
CBZ III-NIC mixture
CBZ-SAC cocrystal
CBZ III-SAC mixture
CBZ-CIN cocrystal
CBZ III-CIN mixture

(b)

Fig. S5 DSC thermographs of solid residues retrieved from different formulations after dissolution tests (X: no solid residues collected)

	CBZ III	CBZ-NIC cocrystal	CBZ-NIC mixture	CBZ-SAC cocrystal	CBZ-SAC mixture	CBZ-CIN cocrystal	CBZ-CIN mixture
100mg HPMCAS	X		X		X		
200mg HPMCAS	X		X				
100mg PVP	X		X	X	X		

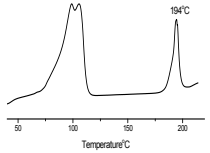
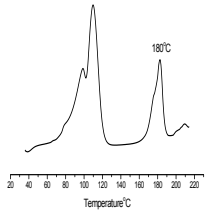
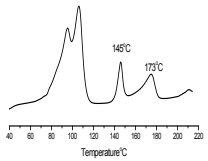
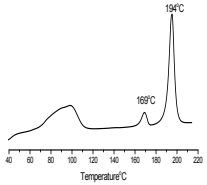
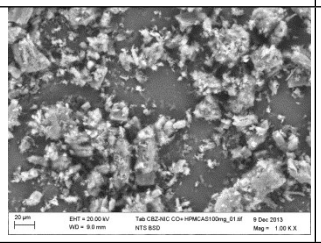
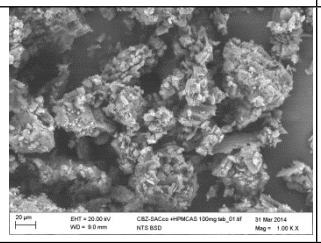
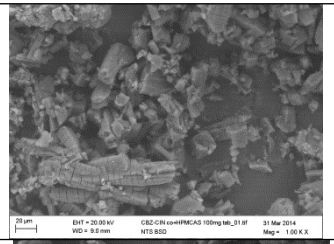
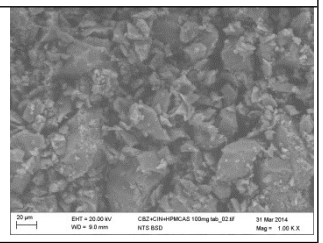
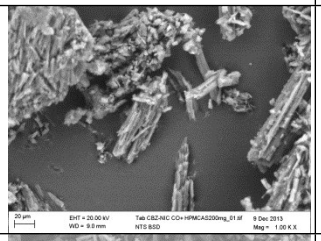
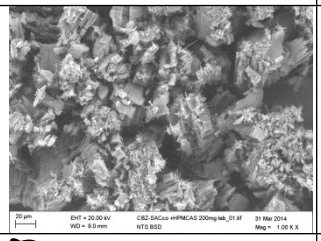
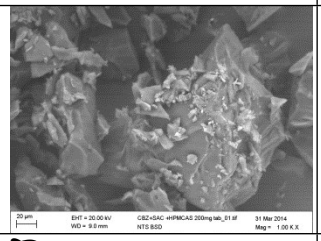
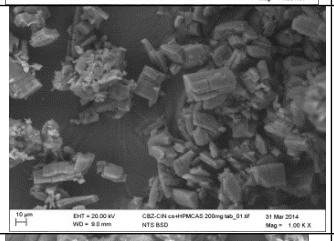
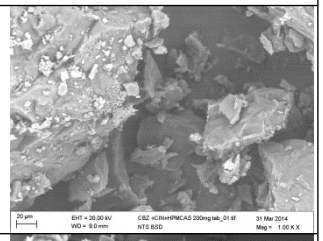
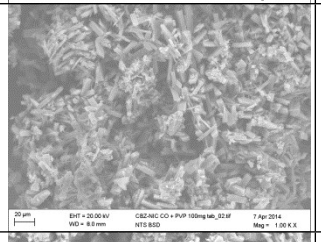
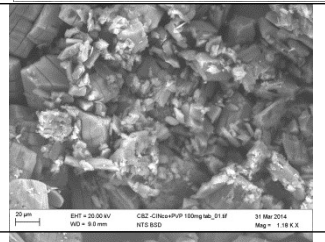
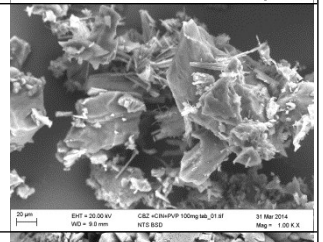
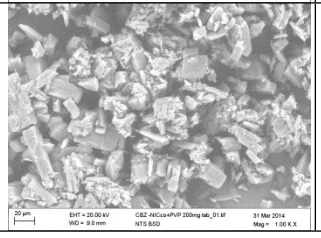
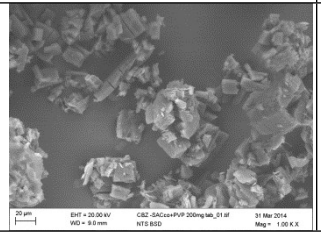
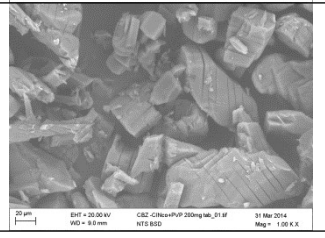
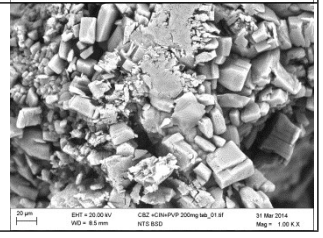
200mg PVP	∅		∅		∅		
100mg PEG	∅	∅	∅	∅	∅	∅	∅
200mg PEG	∅	∅	∅	∅	∅	∅	∅

Figure S6. SEM photographs of solid residues of different formulation after dissolution tests (ϕ, no solid residue collected).

	CBZ III	CBZ-NIC cocrystal	CBZ-NIC mixture	CBZ-SAC cocrystal	CBZ-SAC mixture	CBZ-CIN cocrystal	CBZ-CIN mixture
100mg HPMCAS	ϕ		ϕ		ϕ		
200mg HPMCAS	ϕ		ϕ				
100mg PVP	ϕ		ϕ	ϕ	ϕ		
200mg PVP	ϕ		ϕ		ϕ		

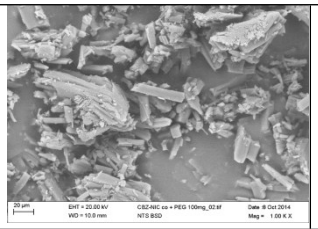
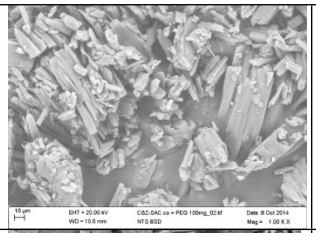
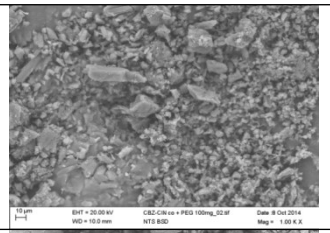
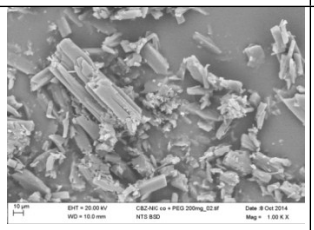
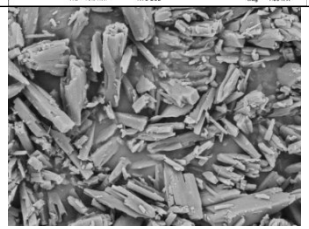
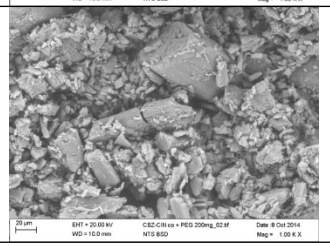
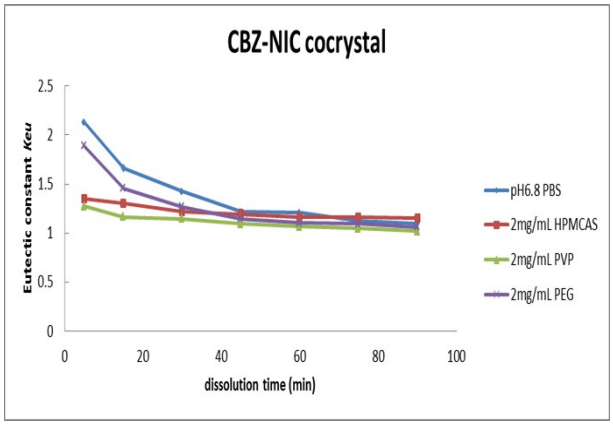
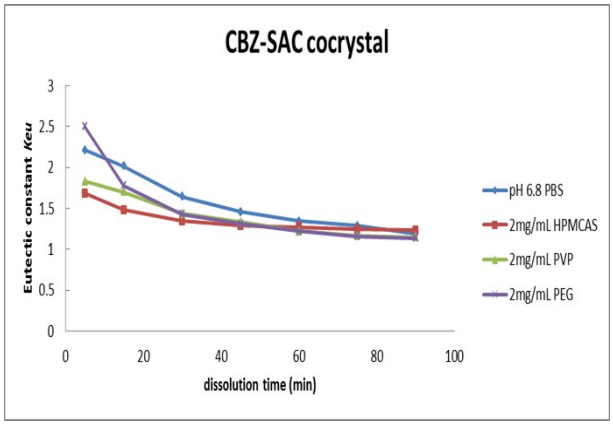
100mg PEG	∅		∅		∅		∅
200mg PEG	∅		∅		∅		∅

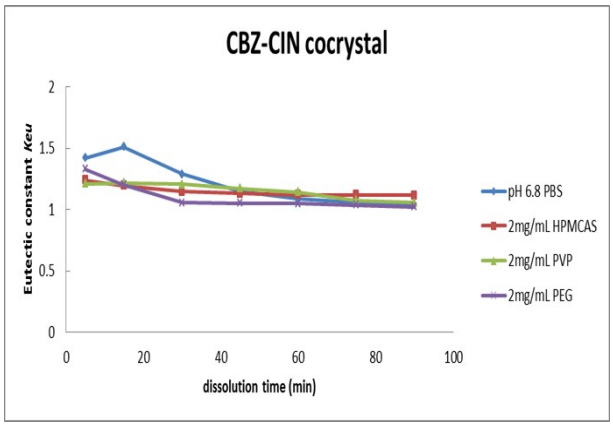
Figure. S6. Eutectic constant K_{eu} of CBZ cocrystals in the absence and presence of a 2 mg/ml polymer in pH6.8 PBS during powder dissolution tests: (a) CBZ-NIC cocrystal; (b) CBZ-SAC cocrystal; (c) CBZ-CIN cocrystal



(a)

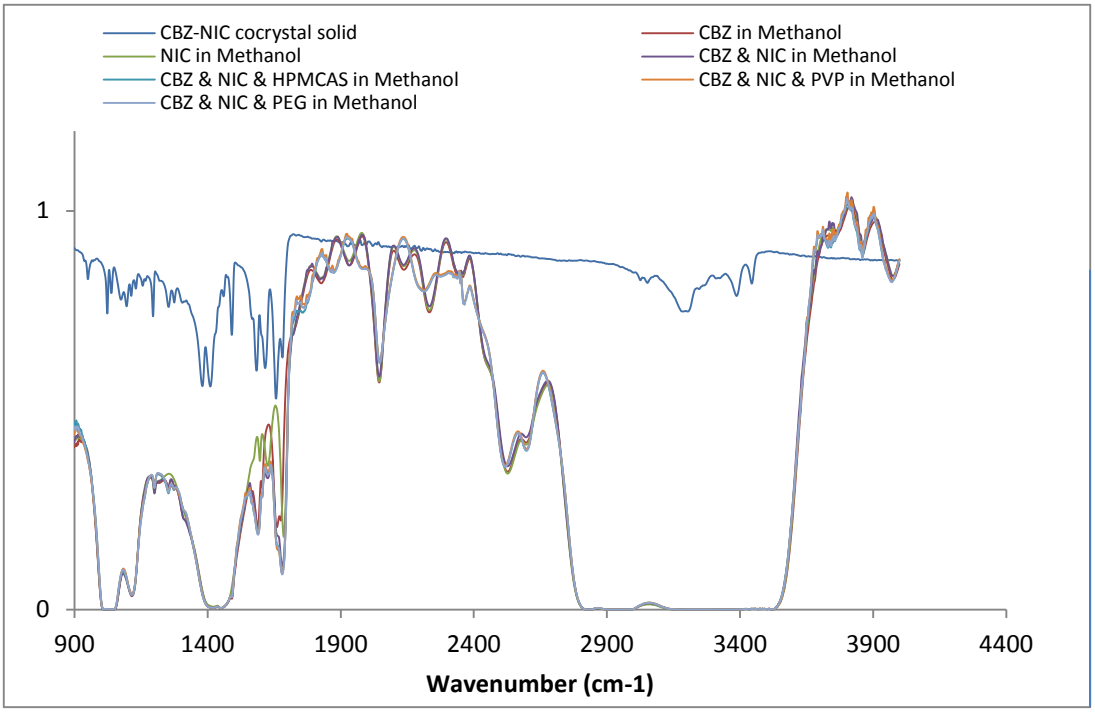


(b)

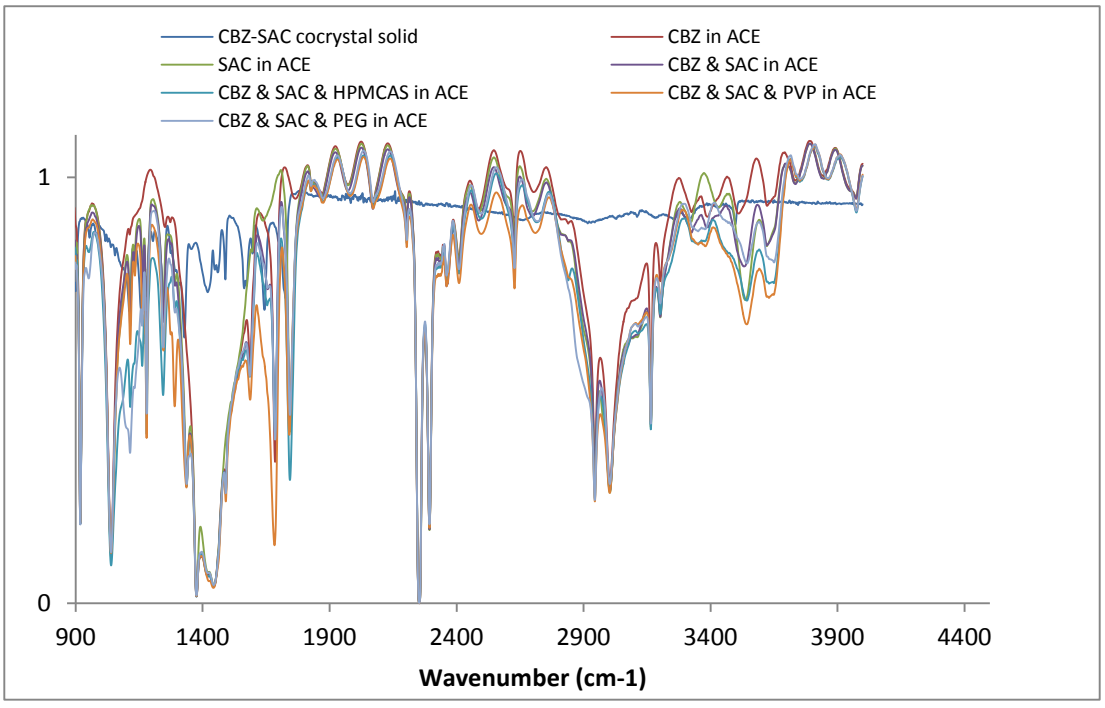


(c)

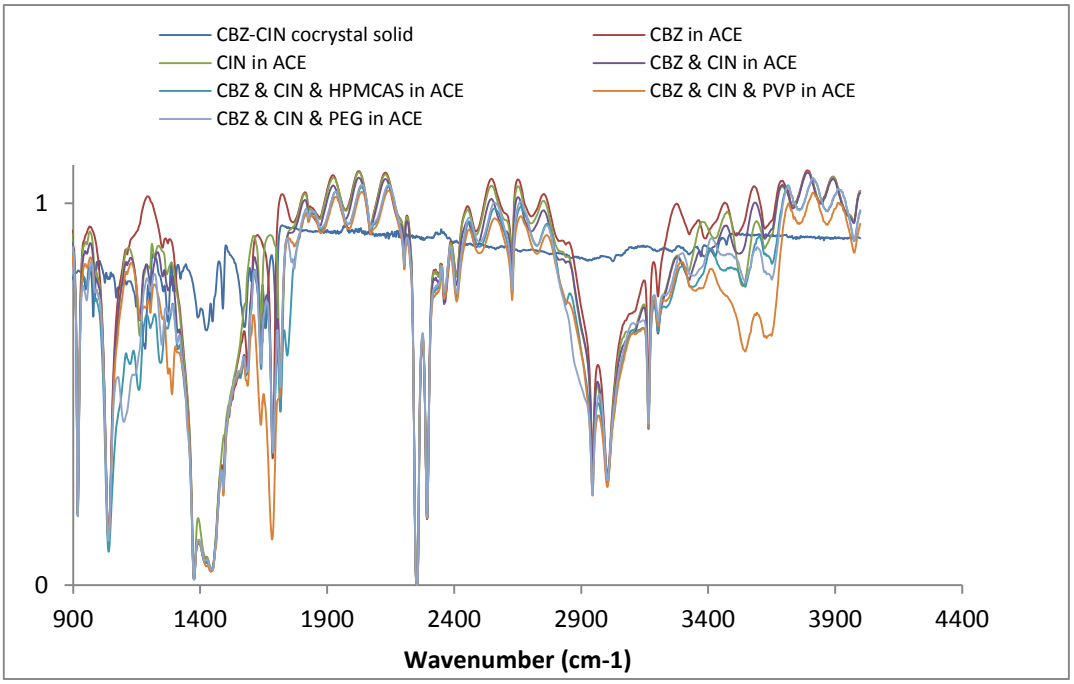
Figure S7. IR spectra: (a) comparison of CBZ-NIC cocrystal solids with individual components and mixture in solution in absence and presence of polymers; (b) comparison of CBZ-SAC cocrystal solids with individual components and mixture in solution in absence and presence of polymers; (c) comparison of CBZ-CIN cocrystal solids with individual components and mixture in solution in absence and presence of polymers;



(a)



(b)


CBZ-CIN cocrystal solid
CBZ in ACE
CIN in ACE
CBZ & CIN in ACE
CBZ & CIN & HPMCAS in ACE
CBZ & CIN & PVP in ACE
CBZ & CIN & PEG in ACE
1
0
900
1400
1900
2400
2900
3400
3900
4400
Wavenumber (cm-1)

(c)