

## Supplementary information

### **Brexiprazole-Catechol Cocrystal: Structure Elucidation, Excipient Compatibility and Stability**

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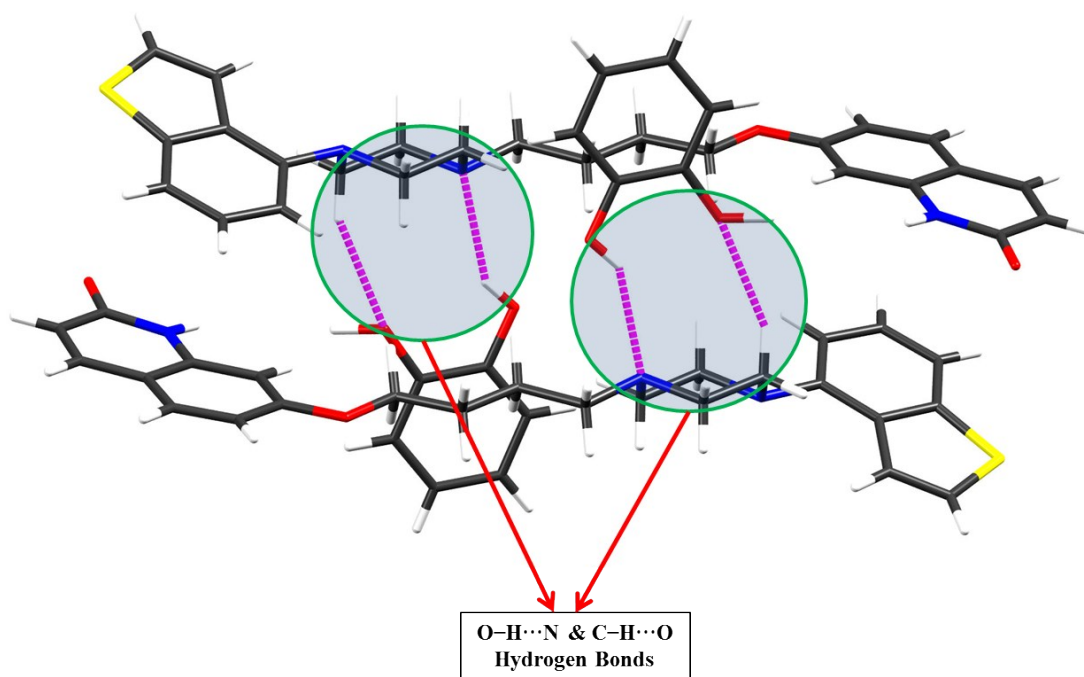
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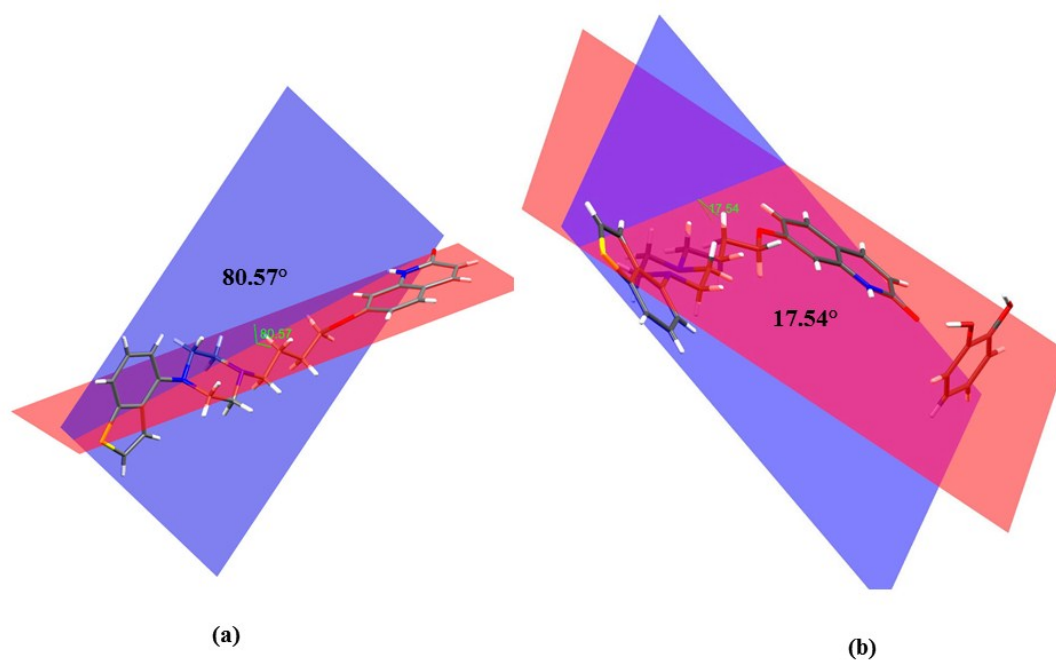
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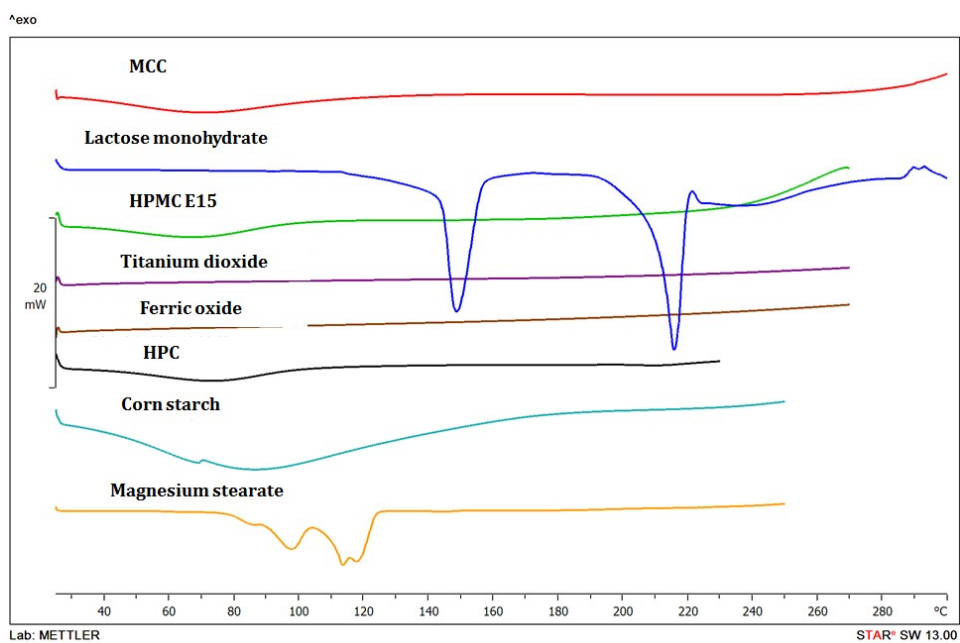
**Address:** Amneal Pharmaceuticals India, 901 – 911, Iscon Elegance, Nr. Hotel Crown Plaza,  
S. G. Highway, Ahmedabad – 380015, Gujarat, India



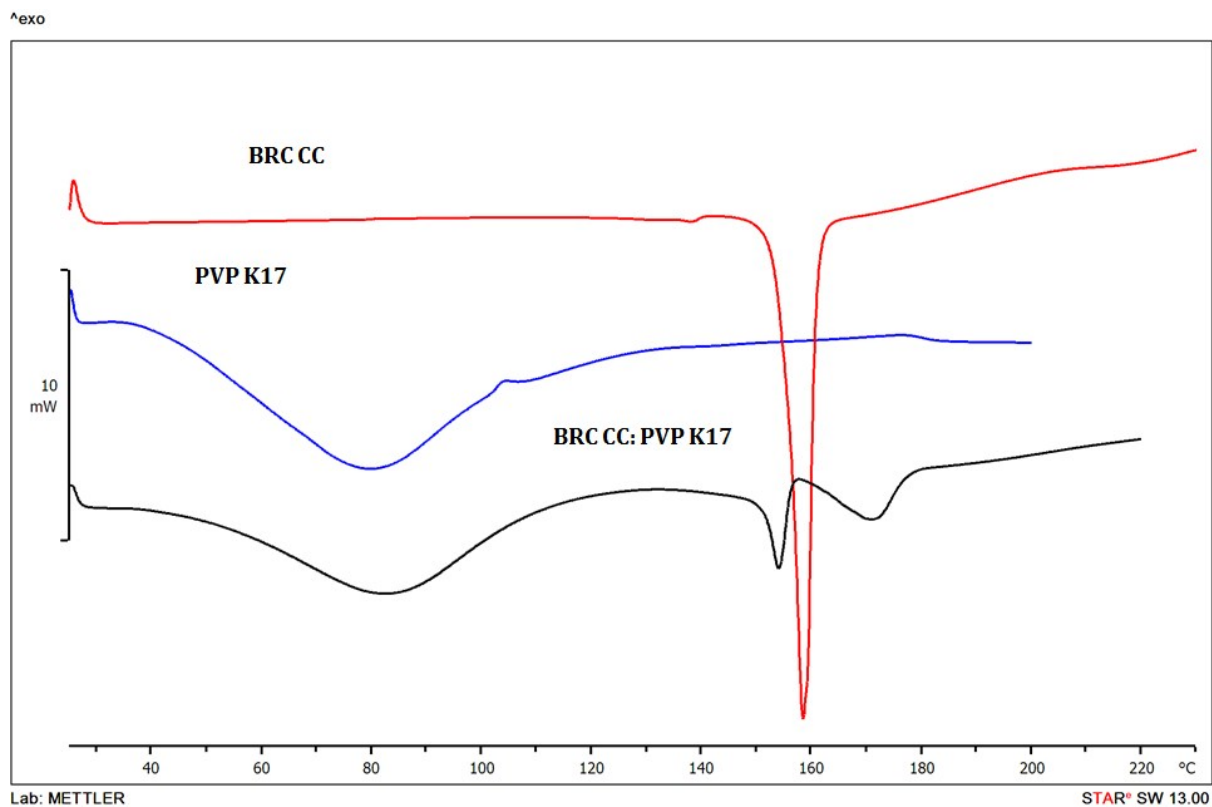
**Figure S1** Representation of hydrogen bonding interactions between BREX and CAT cocrystals.



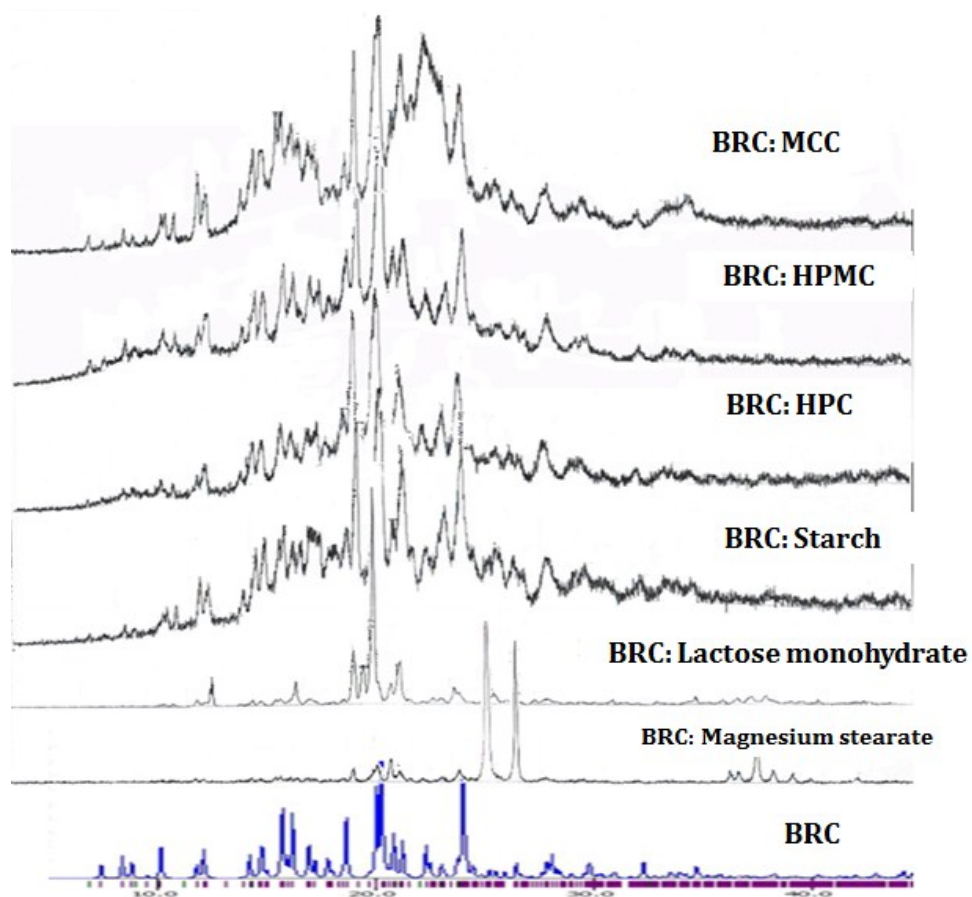
**Figure S2** Representation of conformation angle change between two planer carbostyryl and benzothiaphene.



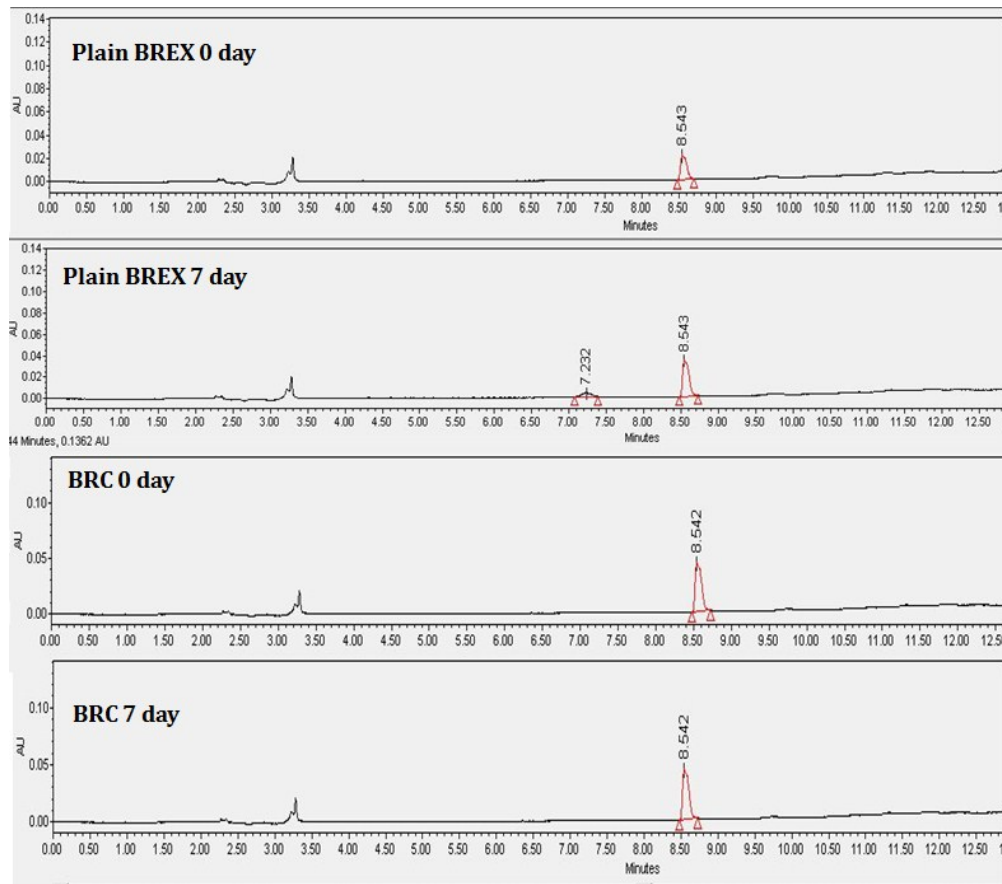
**Figure S3** DSC curves of plain excipients



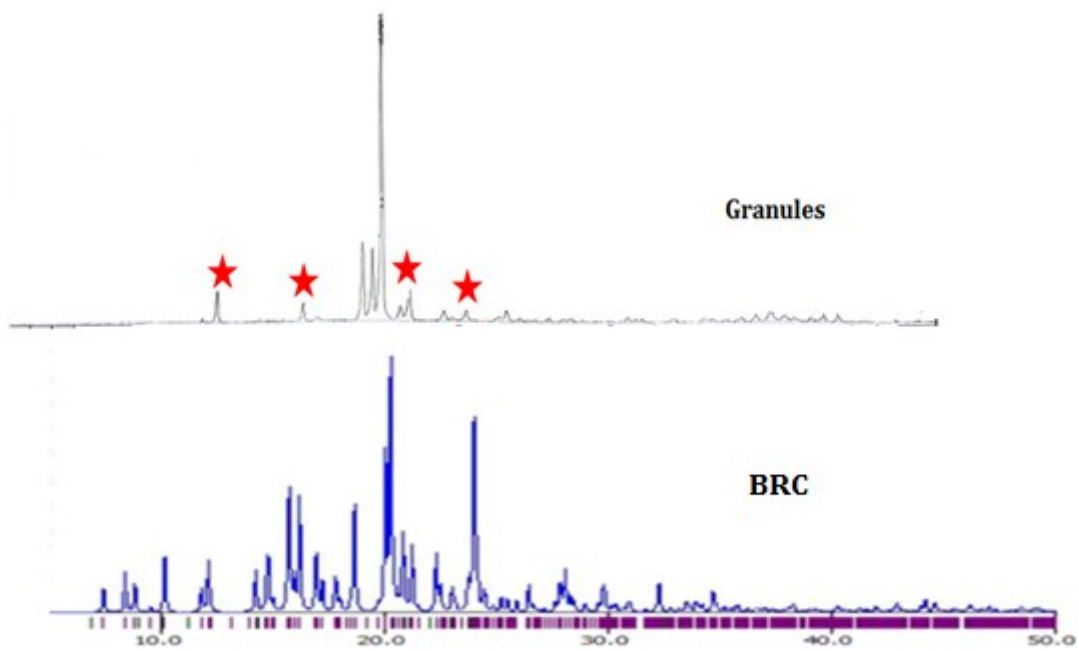
**Figure S4** DSC curves of BRC cocrystal (CC), PVP K17 and physical mixture of cocrystal and PVP K17



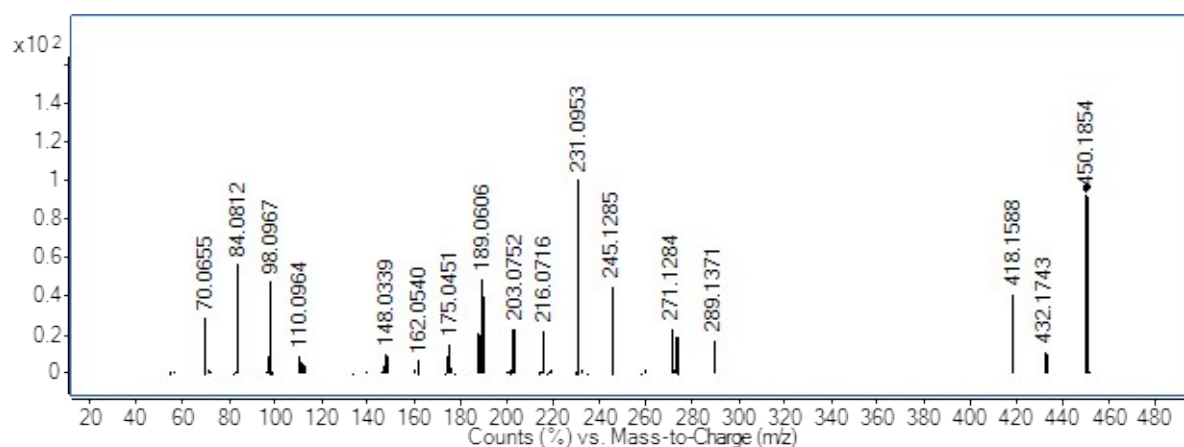
**Figure S5** PXR overlay of excipient compatibility samples with simulated XRD of BRC cocrystal



**Figure S6** HPLC chromatograms of BREX and BRC cocrystal before and after stability study



**Figure S7** PXRD overlay of granules and simulated XRD pattern of BRC cocrystal



**Figure S8** Mass spectrum of N-oxide impurity of BREX

**Table S1** HPLC parameters

HPLC Parameter	Optimized values	Gradient program		
		Time	Aqueous content (v/v)	Organic content (v/v)
Mobile phase	Acetonitrile and 10 mM ammonium formate adjusted to pH 4.2 with 0.1N formic acid	0	50	50
Elution	Gradient	3	40	60
Flow rate	1 ml/min	6	30	70
Wavelength	270 nm	9	15	85
Injection volume	10 µl	12	50	50
		16	50	50

**Table S2** Compositions of granules

<b>Granules with plain BREX (%w/w)</b>	<b>Granules with BRC cocrystal (%w/w)</b>
Brexpiprazole (4.10)	Brexpiprazole (5.12)
Microcrystalline cellulose (10.75)	Microcrystalline cellulose (10.75)
Corn starch (21.51)	Corn starch (21.51)
Lactose monohydrate (51.05)	Lactose monohydrate (51.05)
Magnesium stearate (0.65)	Magnesium stearate (0.65)
PVP K17 (1.51)	PVP K17 (1.51)
Titanium dioxide (0.25)	Titanium dioxide (0.25)
Ferric oxide (0.56)	Ferric oxide (0.56)
HPC (6.25)	HPC (6.25)