

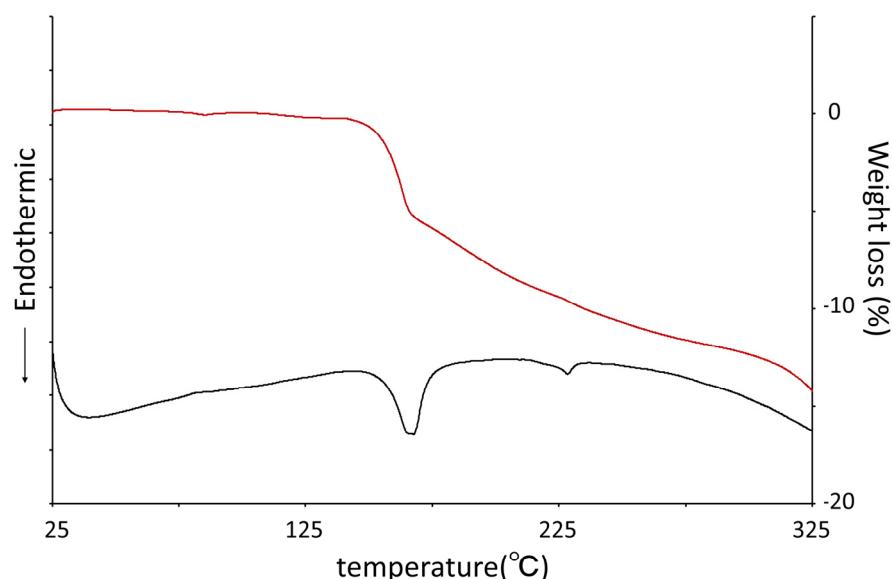
## Electronic Supplementary Information

### Cocrystal Structure Design for CH5134731 Based on Isomorphism

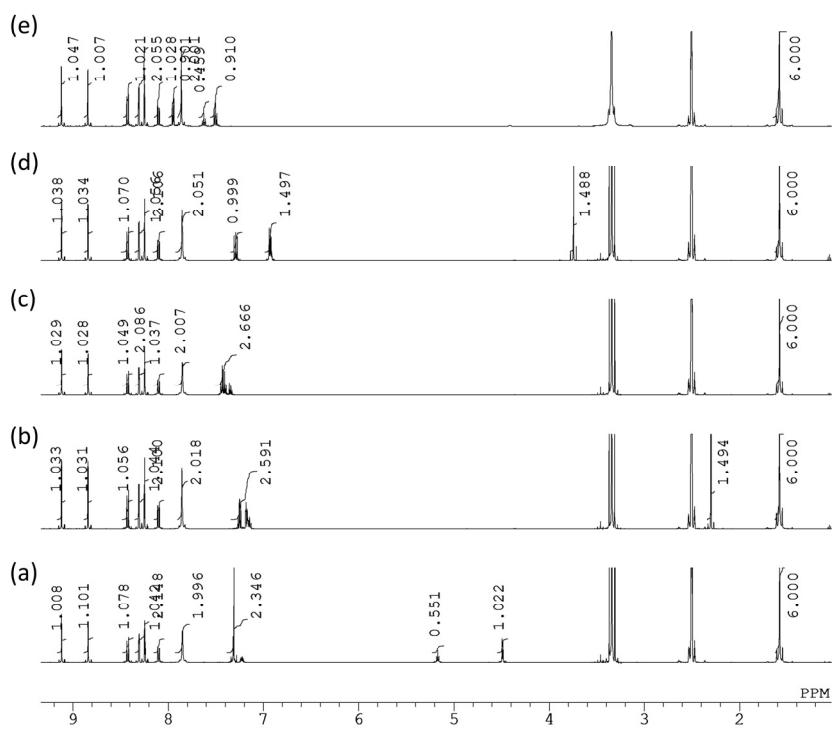
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**Fig. S1.** TG (red) and DTA (black) curves of CH5134731 benzoic acid cocrystal.



**Fig. S2.**  $^1\text{H}$ -NMR (a)benzyl alcohol solvate, (b) toluene solvate, (c) chlorobenzene solvate, (d) anisole solvate, (e) benzoic acid cocrystal