Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Investigating solubilization effect of oxcarbazepine by forming cocrystals

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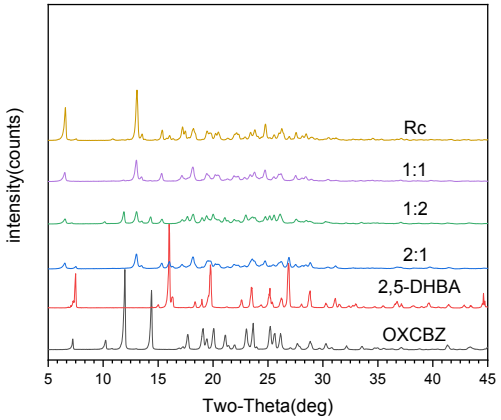
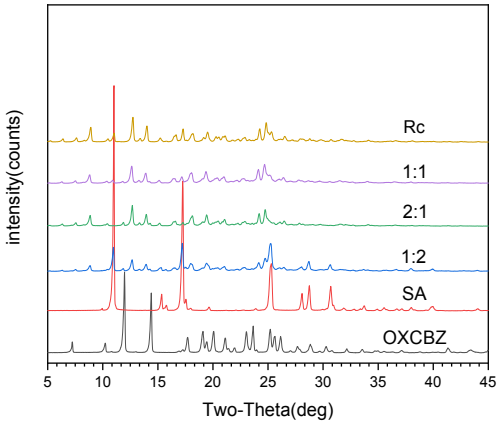
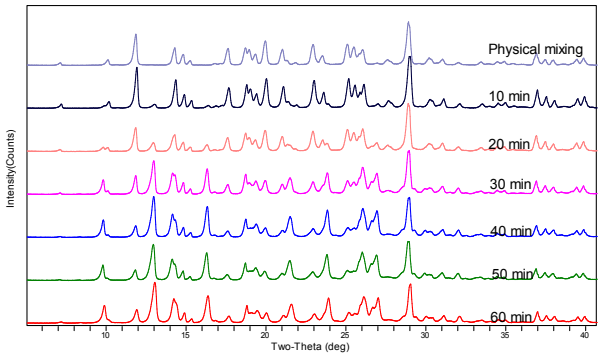


(a)

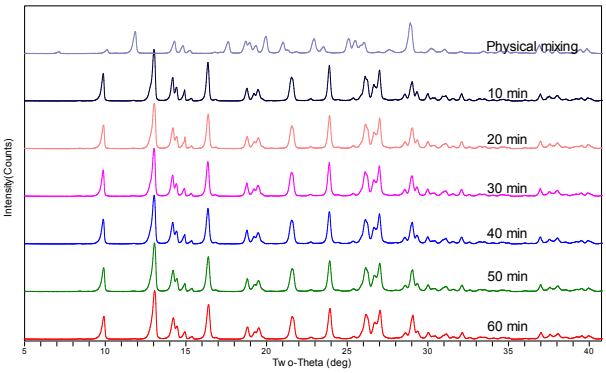


(b)

Fig. **S1** PXRD patterns of co-crystals (a) OXCBZ-2,5-DHBA and (b) OXCBZ-SA.

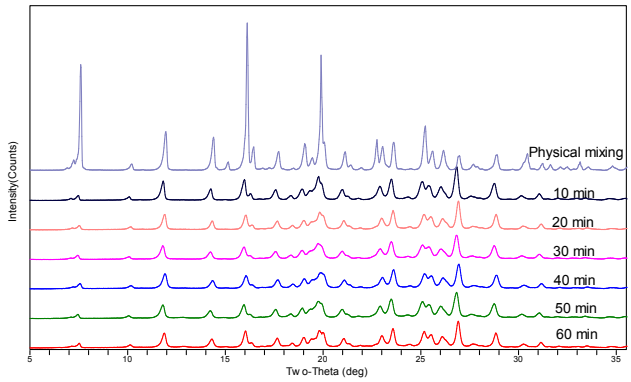


(a)

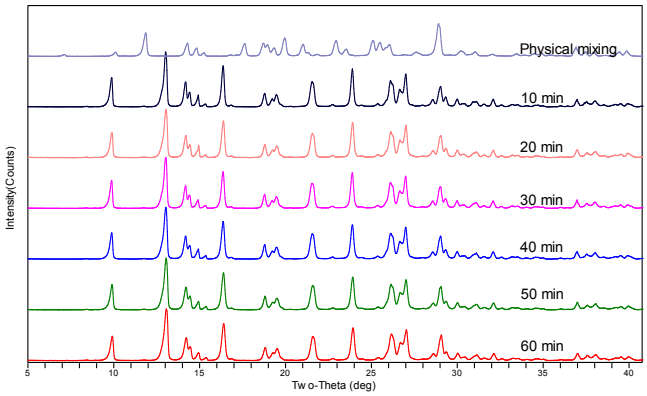


(b)

Fig. **S2** PXRD patterns of OXCBZ-OA cocrystals formed by different methods. (a) grinding by NG and (b) grinding by LAG.

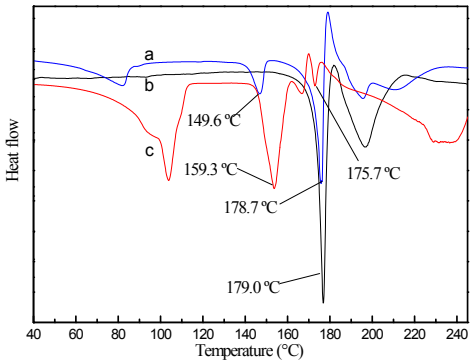


(a)

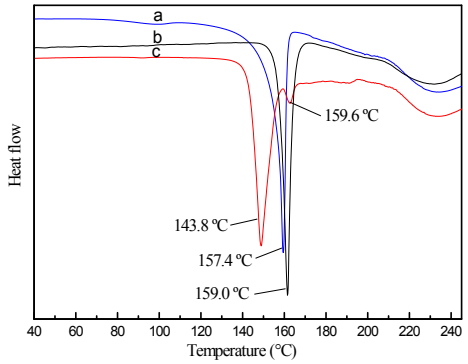


(b)

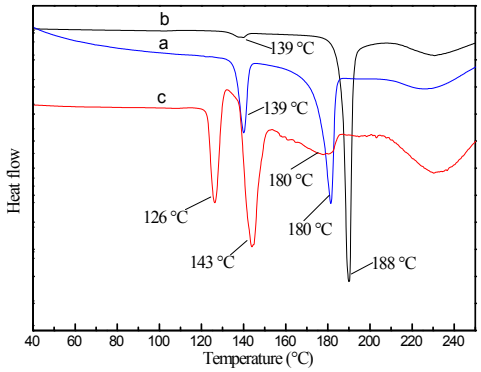
Fig. **S3** PXRD patterns of OXCBZ-2,5-DHBA cocrystals formed by different methods. (a) grinding by NG and (b) grinding by LAG.



OXCBZ-OA



OXCBZ-2,5-DBHA



OXCBZ-SA

Fig. **S4** DSC curves of cocrystals formed under different conditions. (a) LAG, (b) RC and (c) physical mixing.

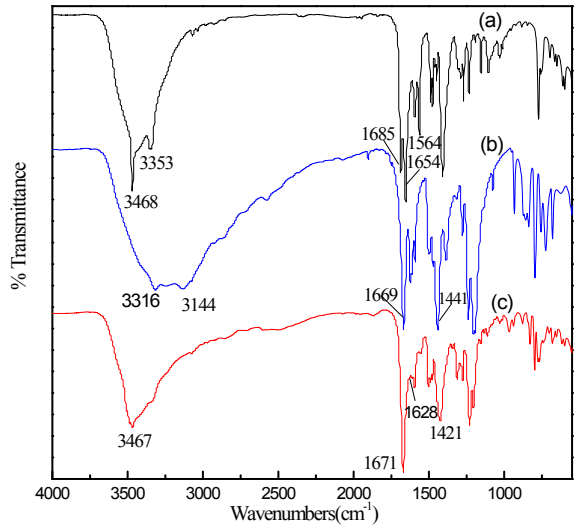


Fig. **S5** FT-IR spectra of OXCBZ and its cocrystal. (a) OXCBZ, (b) 2,5-DHBA and (c) OXCBZ-2,5-DHBA cocrystal.

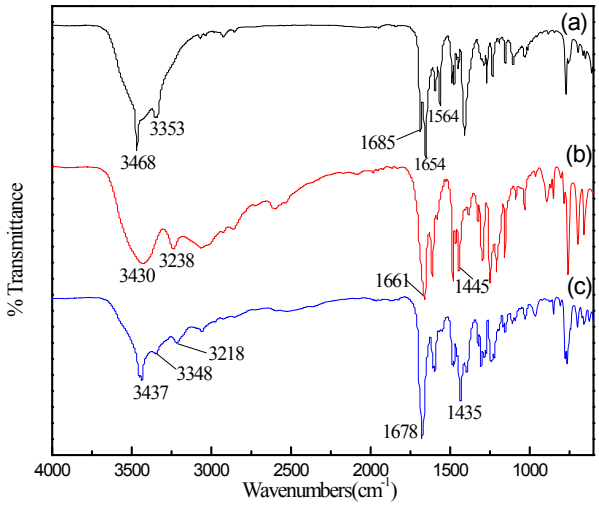


Fig. **S6** FT-IR spectra of OXCBZ and its cocrystals (a) OXCBZ, (b) SA and (c) OXCBZ-SA cocrystal.

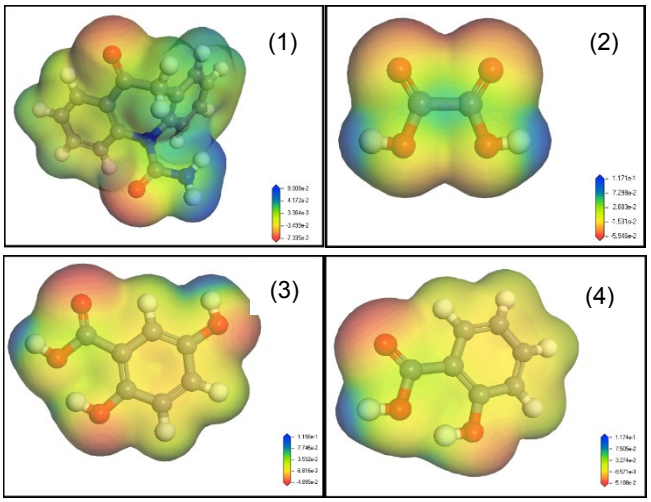


Fig. **S7** Surface electrostatic potentials of (1) OXCBZ, (2) OA, (3) 2,5-DHBA and (4) SA.

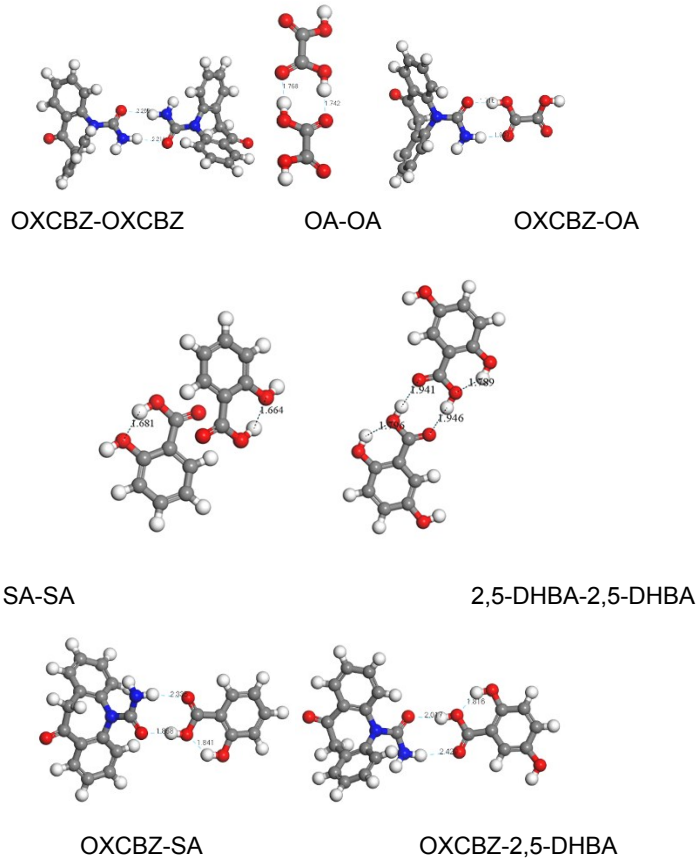
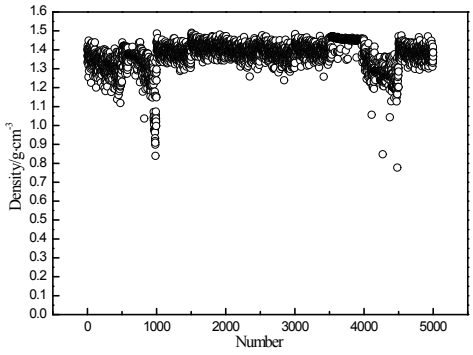
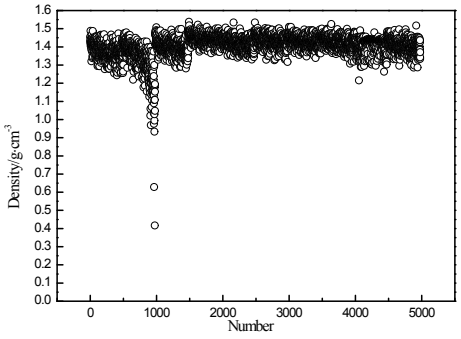


Fig. **S8** Geometric structure diagrams after the basic group optimization.



(a)



(b)

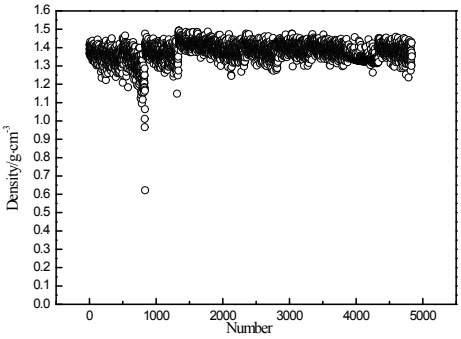
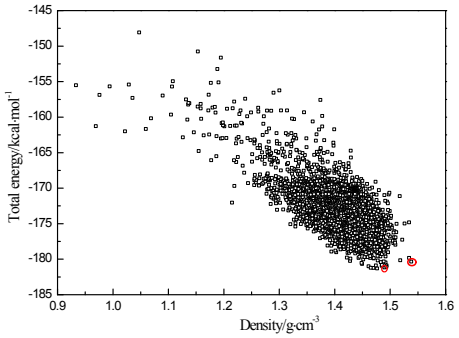
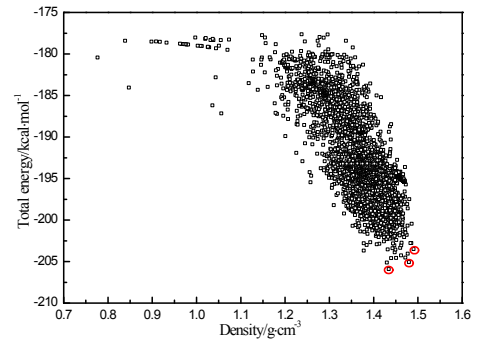


Fig. **S9** Density distribution of cocrystals (a) OXCBZ-OA cocrystal, (b) OXCBZ-2,5-DHBA cocrystal and (c) OXCBZ-SA cocrystal.



(a)



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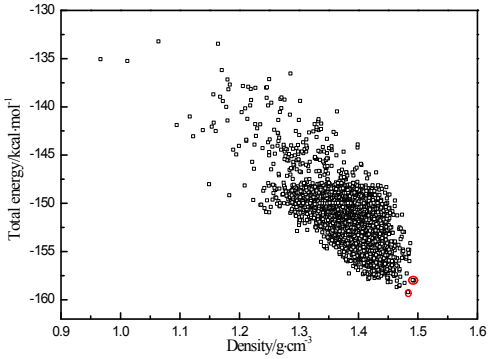


(c)

Fig. **S10** Energy and density distributions of cocrystals (a) OXCBZ-2,5-DHBA, (b) OXCBZ-OA and (c) OXCBZ-SA.

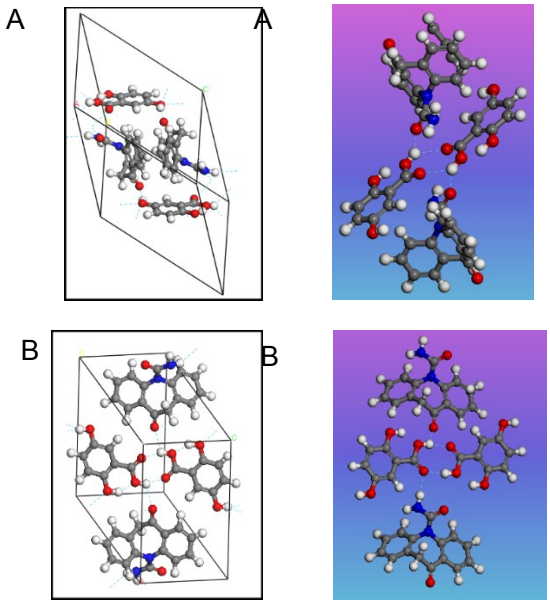


Fig. **S11** Molecular arrangement (left) and H bond position (right) in Unit Cell of OXCBZ-2,5-DHBA cocrystal (A and B correspond to P-1 and P-1 space groups in Table 5, respectively).

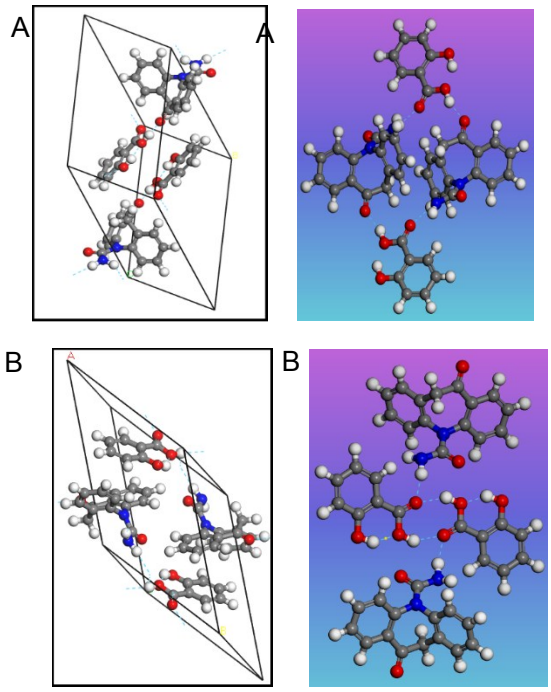
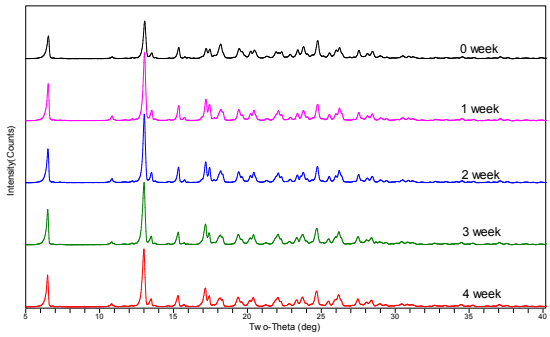
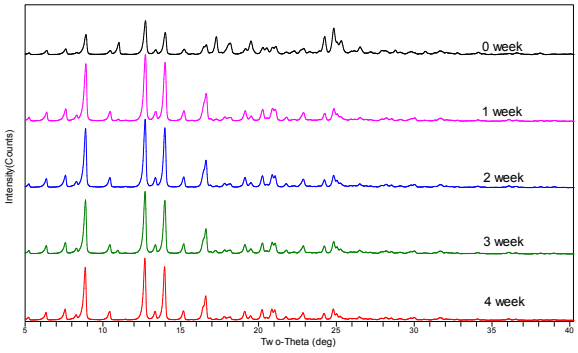


Fig. **S12** Molecular arrangement (left) and H bond position (right) in Unit Cell of OXCBZ-SA cocrystal (A and B correspond to P-1 and P-1 space groups in Table 5, respectively).

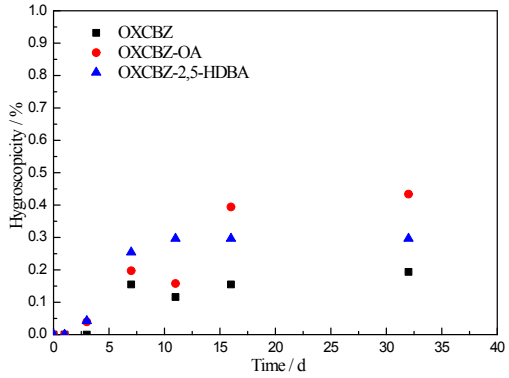


(a)

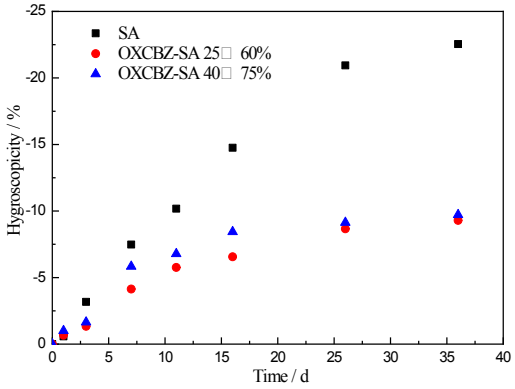


(b)

Fig. **S13.** PXRD patterns of cocrystals at 40 ℃ and different times under 75% RH. (a) OXCBZ-2,5-DHBA cocrystal and (b) OXCBZ-SA cocrystal.



(a) OXCBZ, OXCBZ -OA, and OXCBZ -2,5-DHBA cocrystal at 40 °C, 75% RH



(b) SA and OXCBZ -SA cocrystal at 25 °C, 60% RH and 40 °C, 75% RH

Fig. **S14.** Moisture absorption rates of OXCBZ and its cocrystals.

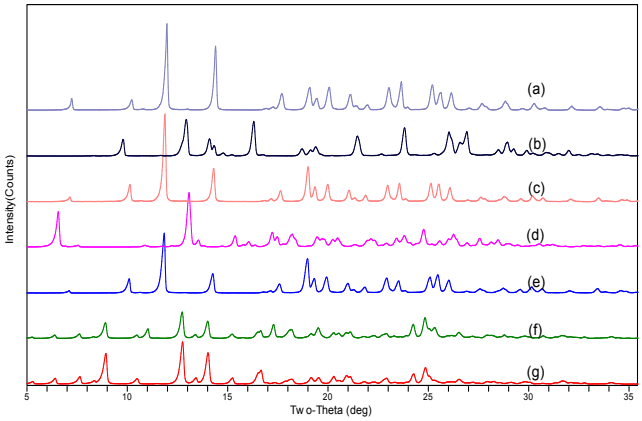


Fig. **S15** PXRD patterns of remaining solid after dissolution of OXCBZ and its cocrystals. (a) OXCBZ, (b) OXCBZ-OA, (c) OXCBZ-OA after dissolution, (d) OXCBZ-2,5-DHBA, (e) OXCBZ-2,5-DHBA after dissolution, (f) OXCBZ-SA and (g) OXCBZ-SA after dissolution.