Supporting Information

Investigating solubilization effect of oxcarbazepine by forming cocrystals

Xiangrong Li,* Guojia Yu,* Xinjian Chen,* Lichao He,* Zhiyong Zhou* and Zhongqi Ren* 

*College of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029, People’s Republic of China

Corresponding author: renzq@mail.buct.edu.cn (Zhongqi Ren); Tel: (+86)-10-64433872; zhouzy@mail.buct.edu.cn (Zhiyong Zhou)

Fig. S1 PXRD patterns of co-crystals (a) OXCBZ-2,5-DHBA and (b) OXCBZ-SA.
Fig. S2 PXRD patterns of OXCBZ-OA cocrystals formed by different methods. (a) grinding by NG and (b) grinding by LAG.
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**
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.
Fig. S9 Density distribution of cocrystals (a) OXCBZ-OA cocrystal, (b) OXCBZ-2,5-DHBA cocrystal and (c) OXCBZ-SA cocrystal.
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).

Fig. S13. PXRD patterns of cocrystals at 40 °C 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.