Supporting Information

Isostructural Cocrystals of Metaxalone with Improved Dissolution Characteristics

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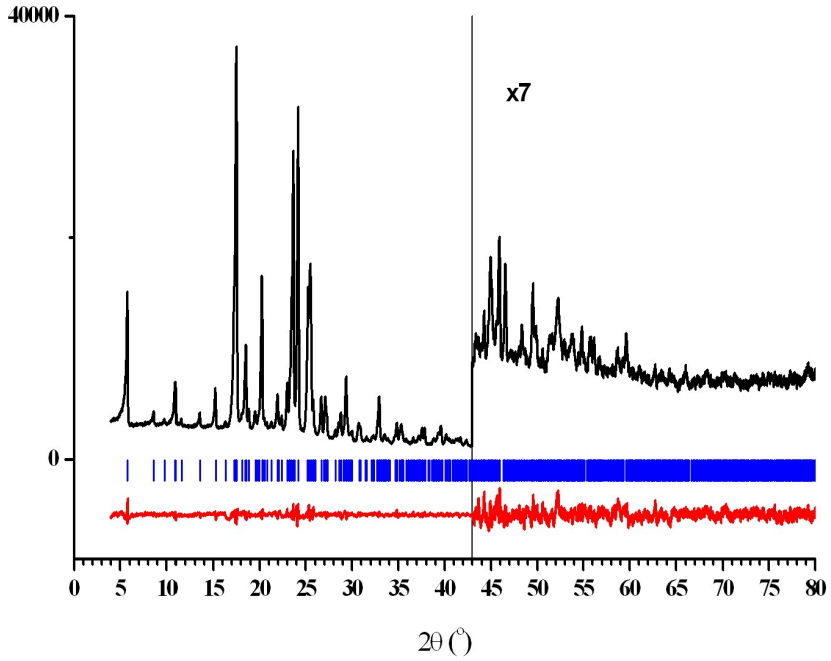
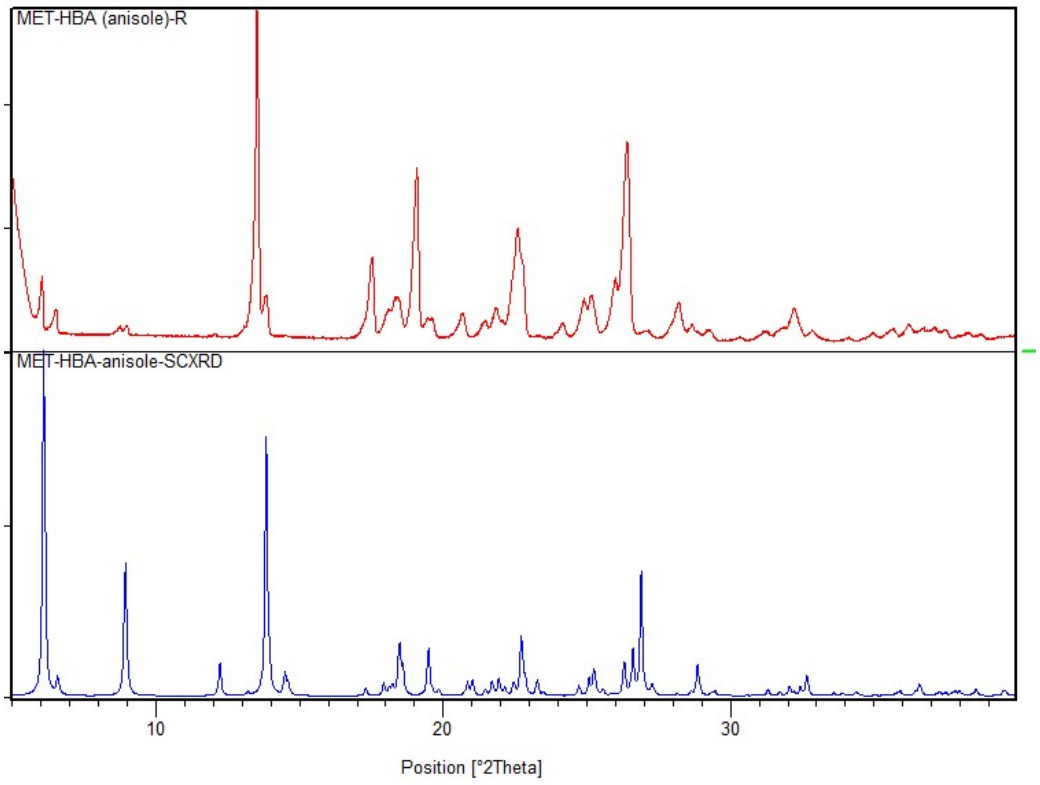


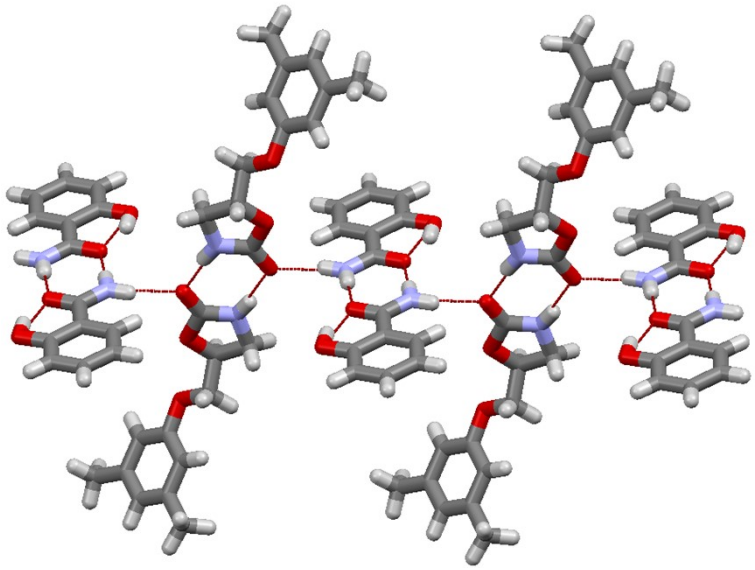
(a)



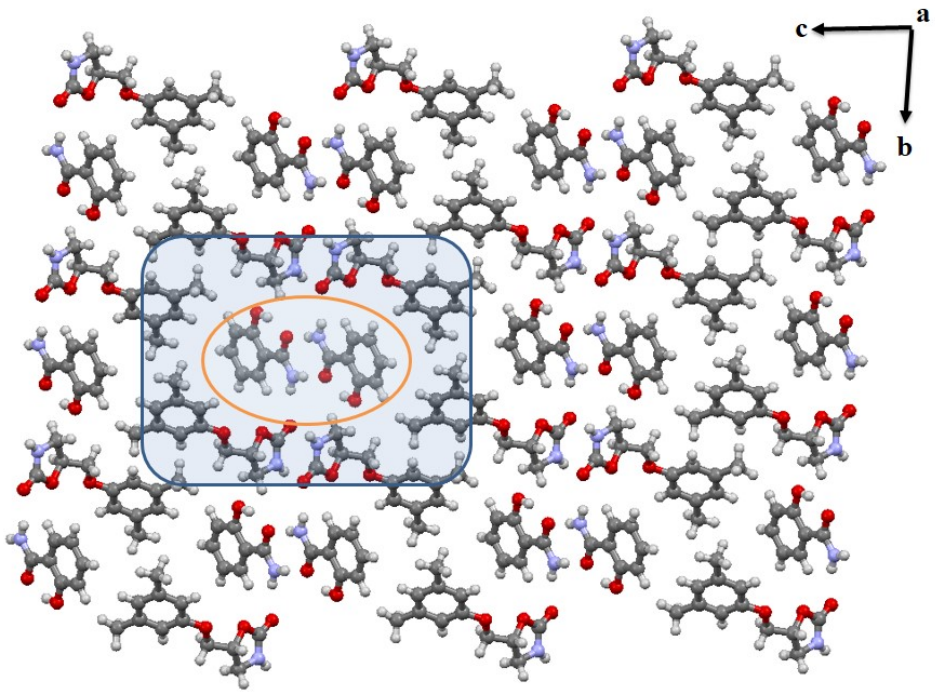
(b)

Fig. S1. (a) The final Rietveld plot for MET–NAM, show the experimental and difference diffraction profiles as black (top) and red (bottom) curves, respectively. The vertical blue bars correspond to the calculated positions of the Bragg peaks. (b) XRD pattern comparison between MET–HBA (anisole)

solvate with its simulated pattern from crystal structure, which suggests except a few diffraction peaks, most of the patterns are matched well.



(a)



(b)

Fig. S2. (a) Hydrogen bonding pattern of MET-SAM cocrystal. (b) 3D packing viewed down the crystallography *a* axis.

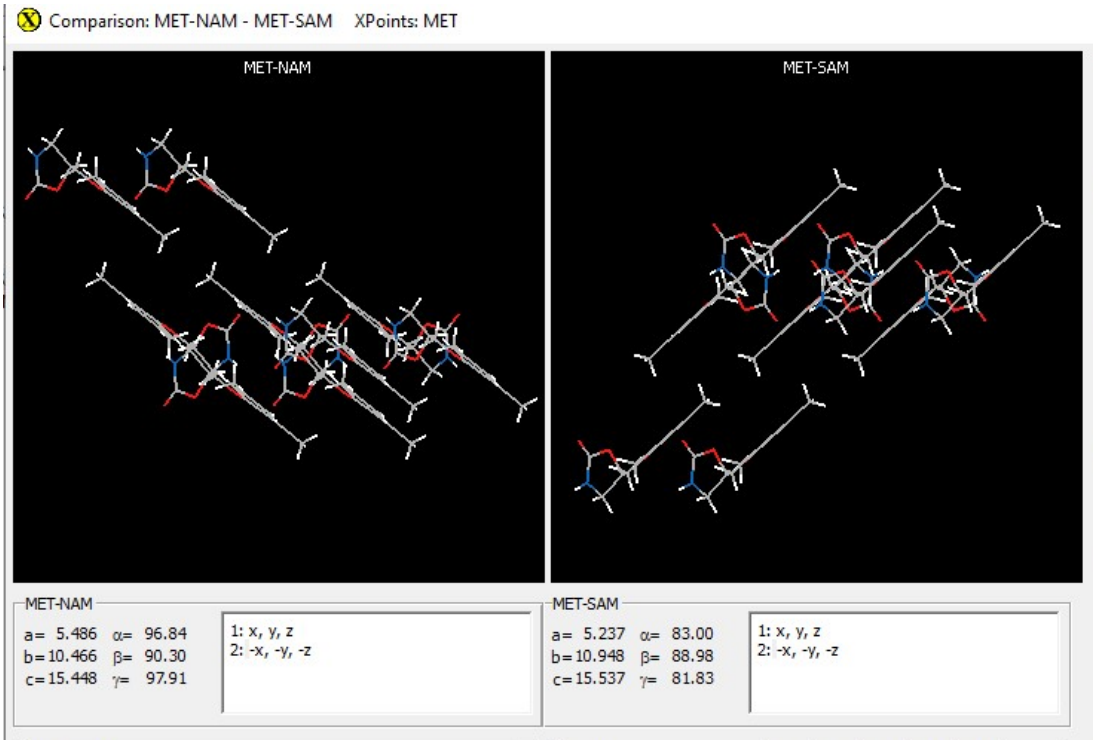


Fig. S3. XPac derived 2D supramolecular constructs of MET–NAM and MET–SAM cocrystals.

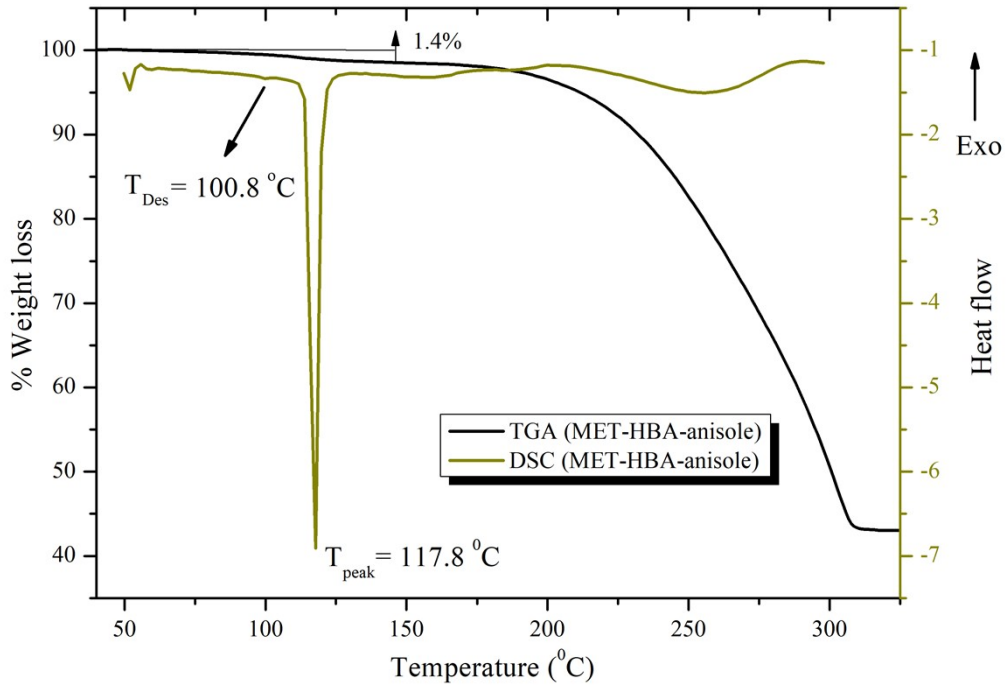
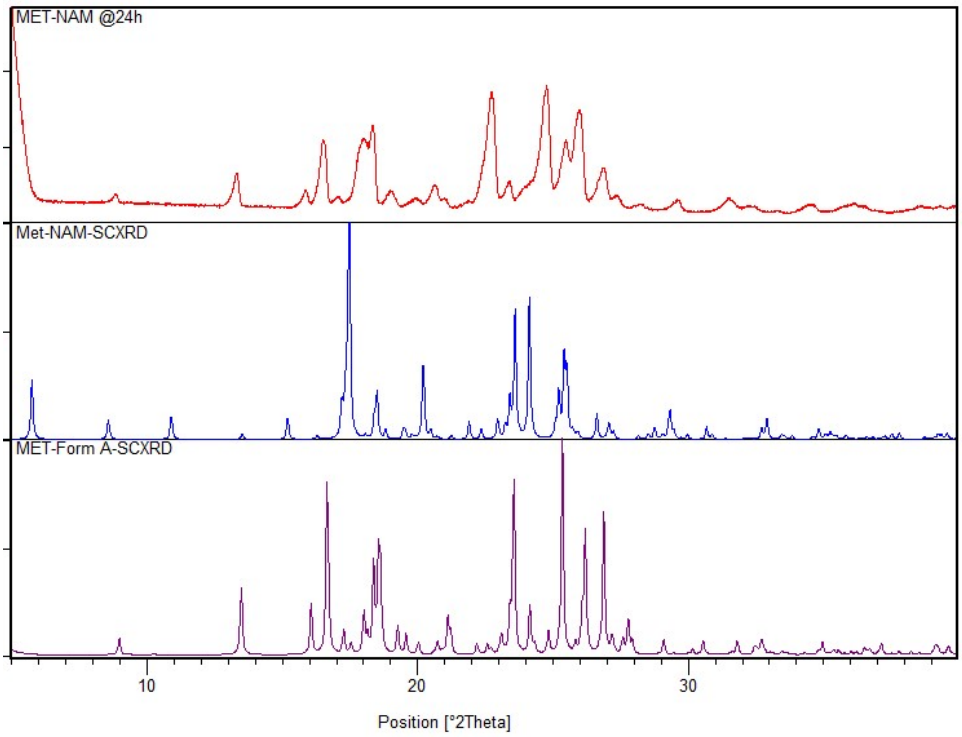
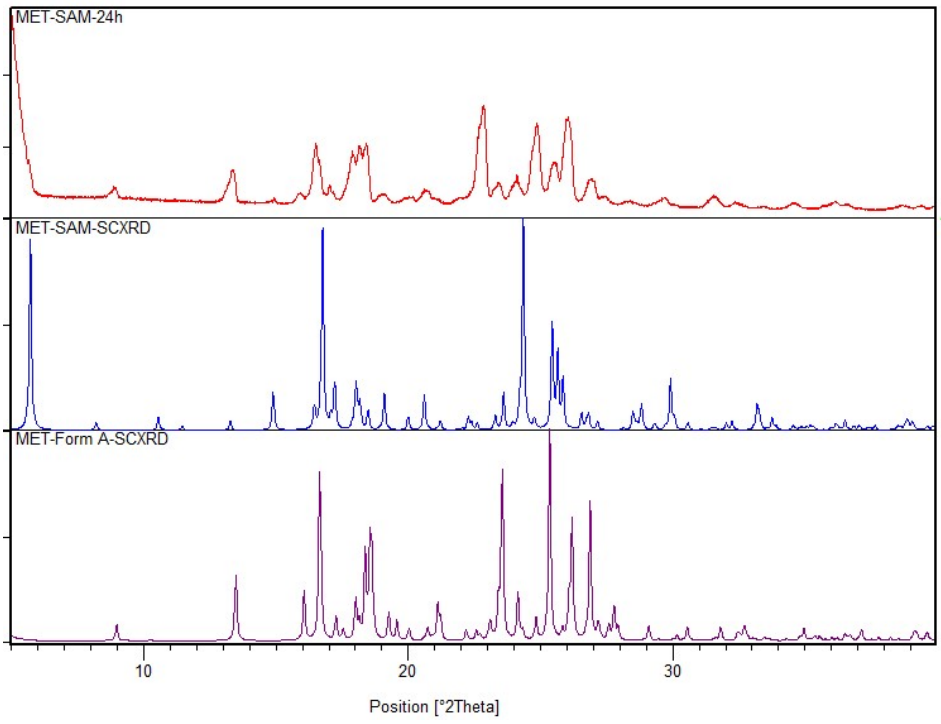


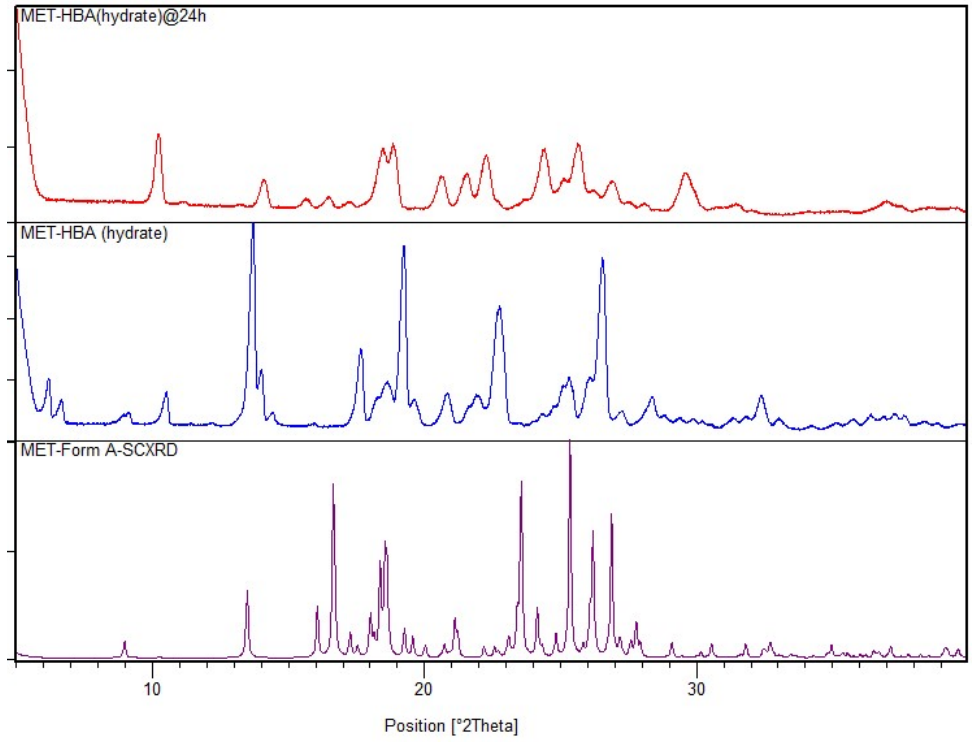
Fig. S4. DSC and TGA comparison of MET–HBA (anisole) solvate after storage for 3 months at ambient conditions indicates the gradual loss of anisole from the cocrystal lattice.


MET-NAM @24h
Met-NAM-SCXRD
MET-Form A-SCXRD
10
20
30
Position [°2Theta]

(a)


MET-SAM-24h
MET-SAM-SCXRD
MET-Form A-SCXRD
10
20
30
Position [°2Theta]

(b)



(c)

Fig. S5. XRD data comparison of (a) MET–NAM, (b) MET–SAM, and (c) MET–HBA (hydrate) with their calculated X-ray patterns and MET (Form I) that confirmed MET–NAM cocrystal transformed to the drug only, whereas MET–SAM and MET–HBA (hydrate) partially transformed to the drug alone.