

Supplementary Information

Isostructurality in Six Celecoxib Co-crystals Introduced by a Solvent Inclusion

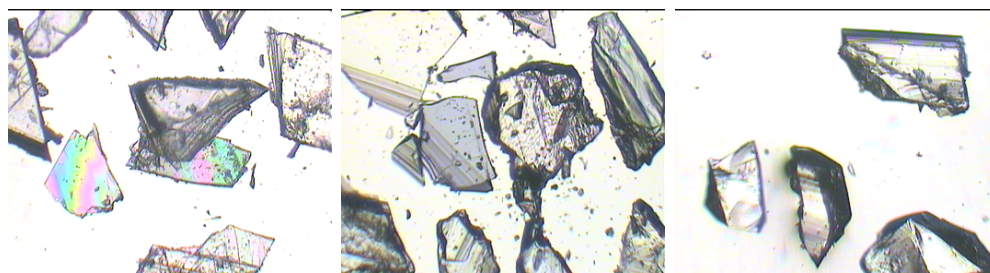
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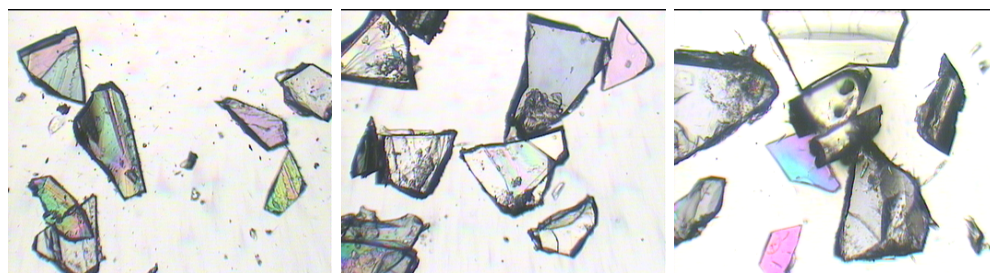
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CEL-BPY (1)

CEL-DPE (2)

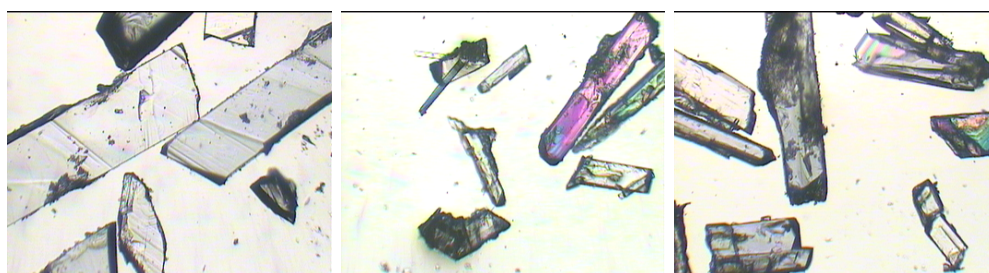
CEL-BPE (3)



S1a

S1b

S1c

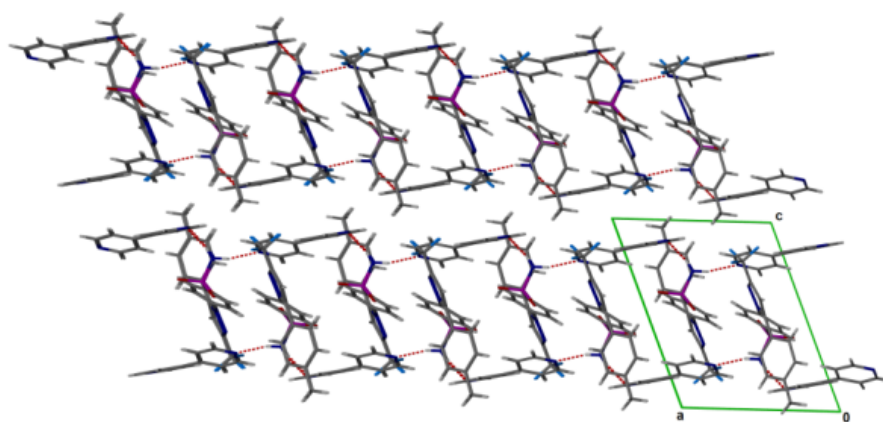


S2a

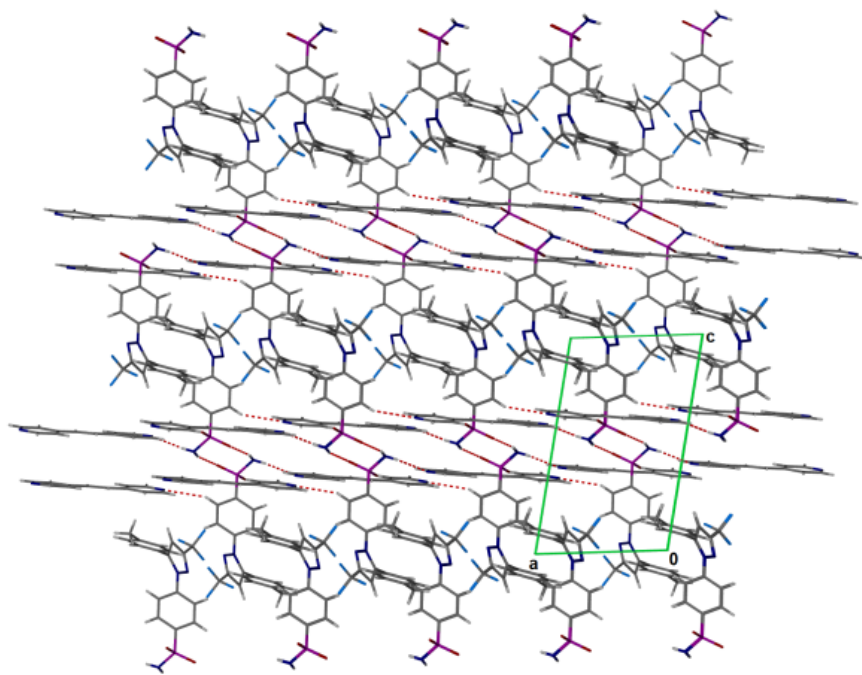
S2b

S2c

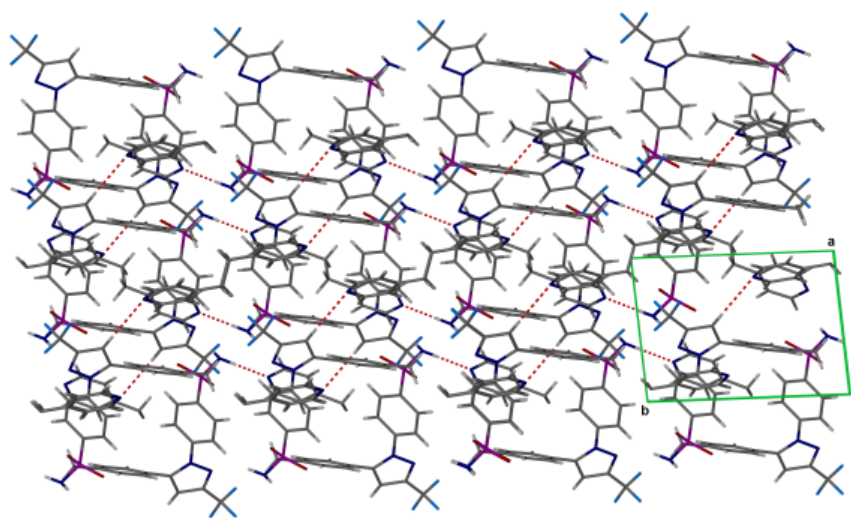
Fig. S1 HSM photographs of CEL unsolvated co-crystals and their solvates



(a)

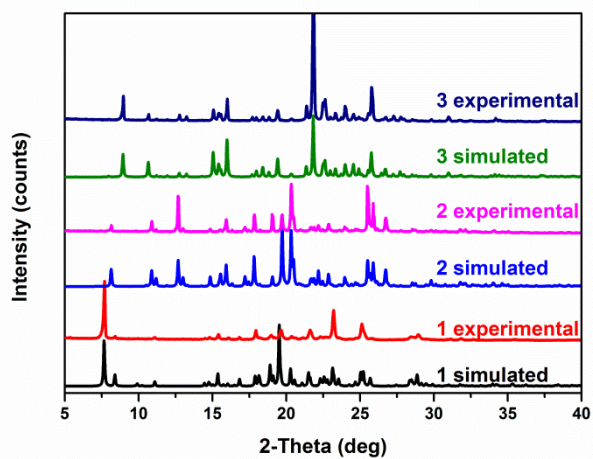


(b)

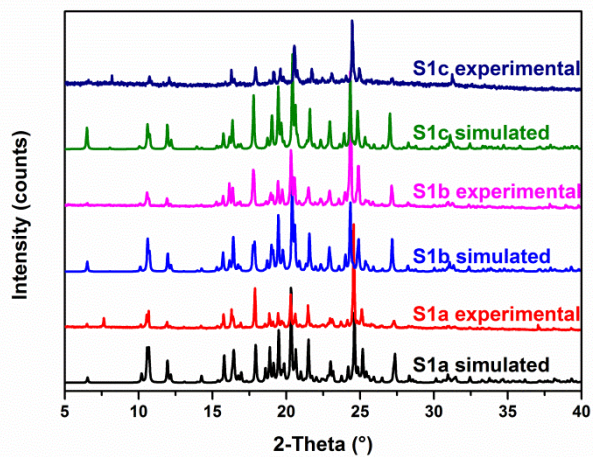


(c)

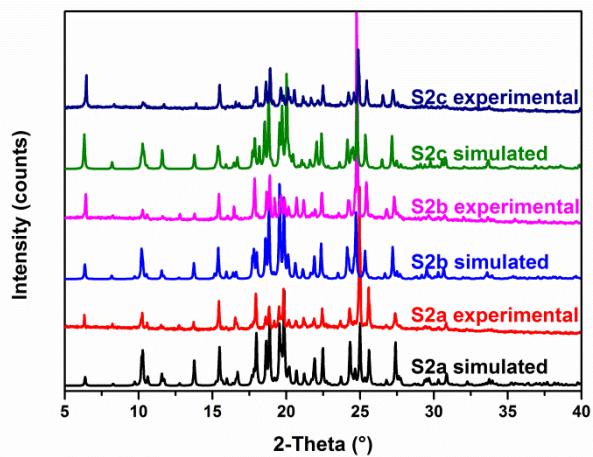
Fig. S2 Distinctive 2D packing structures of (a) CEL-BPY, (b) CEL-DPE, (c) CEL-BPE



(a)



(b)



(c)

Fig. S3 Simulated and experimental XRPD patterns of CEL unsolvated co-crystals and their solvates

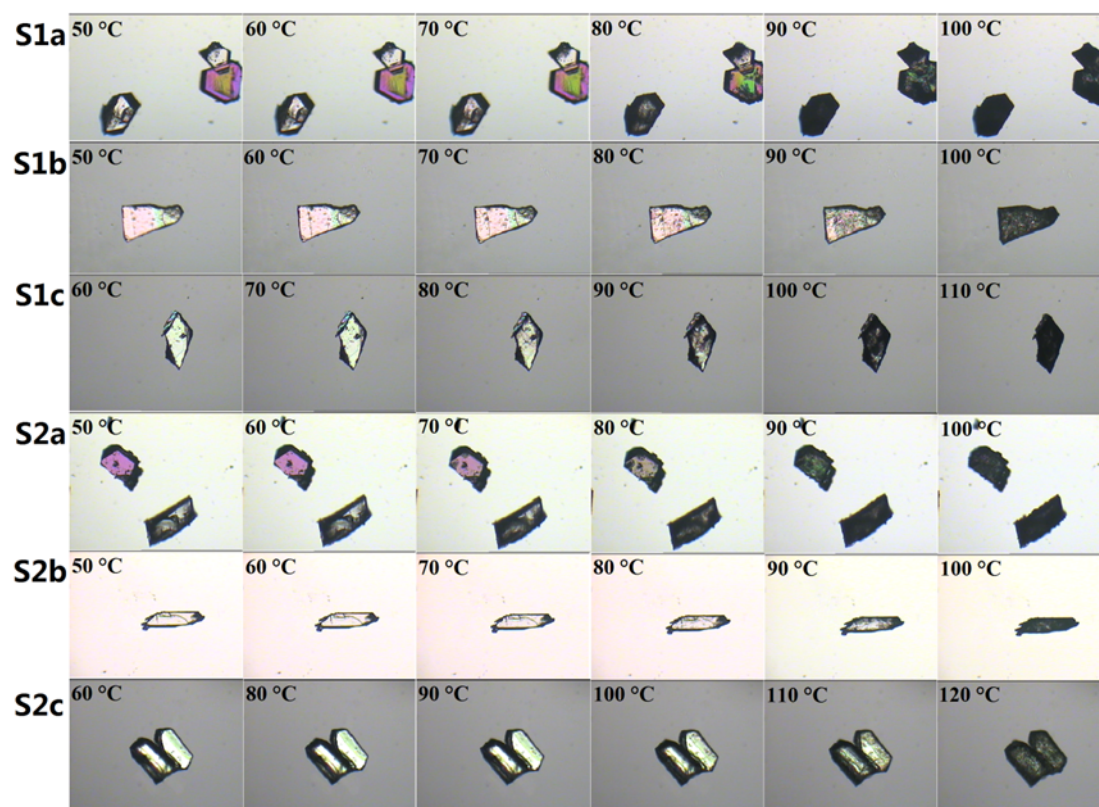
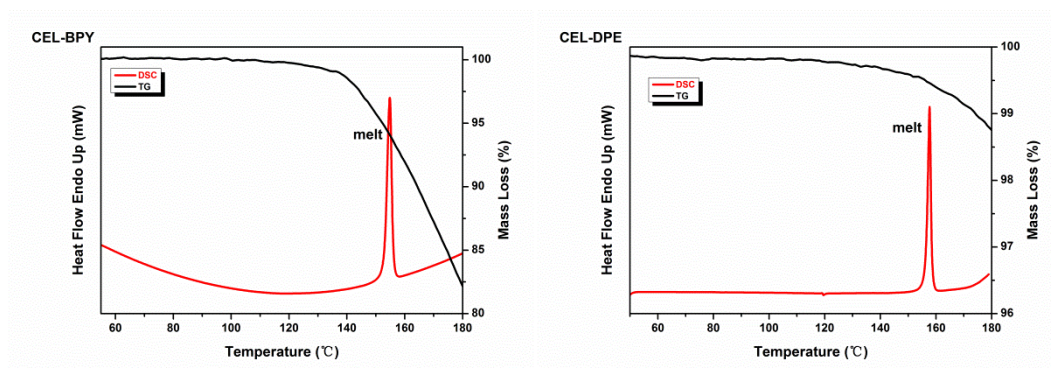


Fig. S4 HSM photographs of six co-crystal solvates at different temperatures



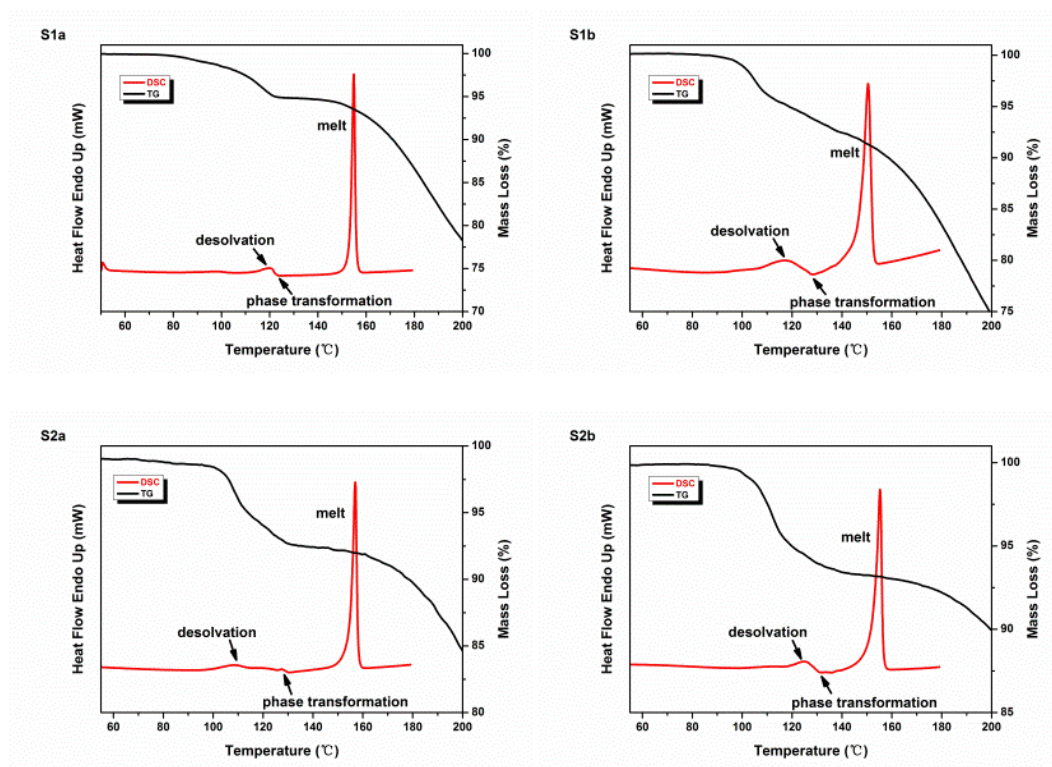
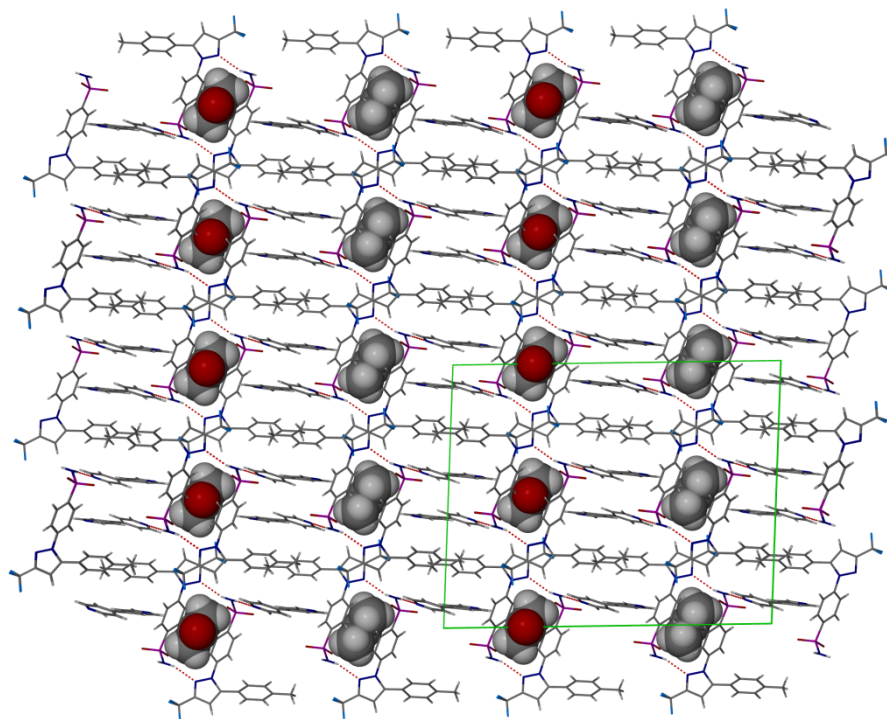
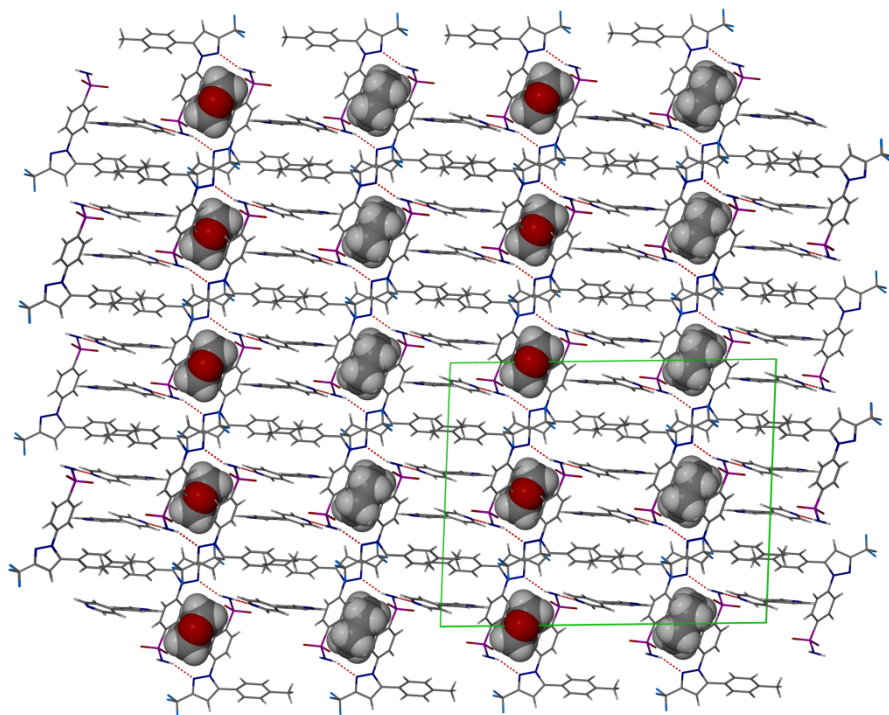


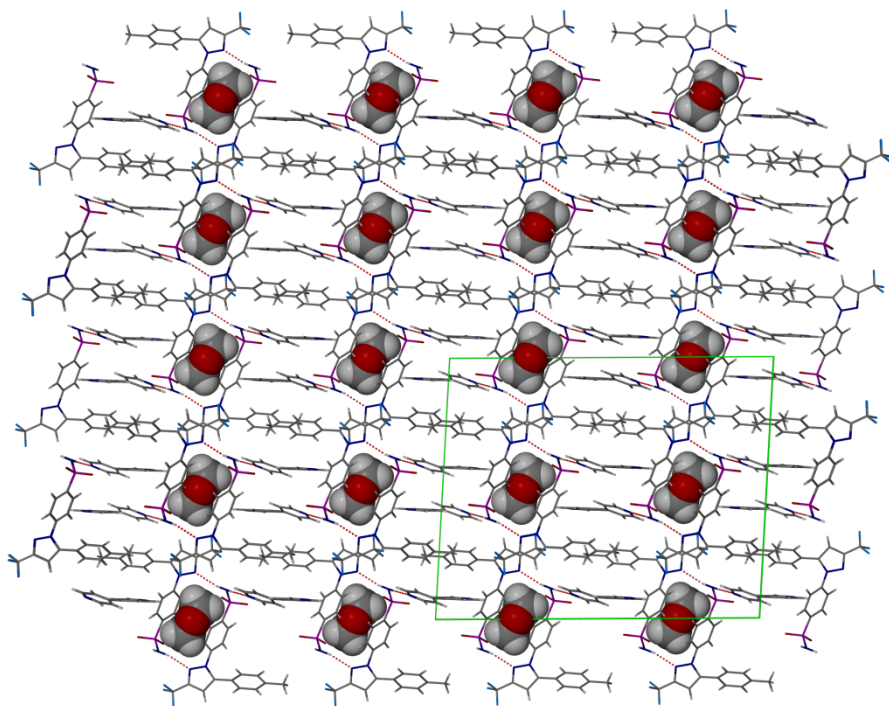
Fig. S5 DSC and TGA thermograms of CEL co-crystals



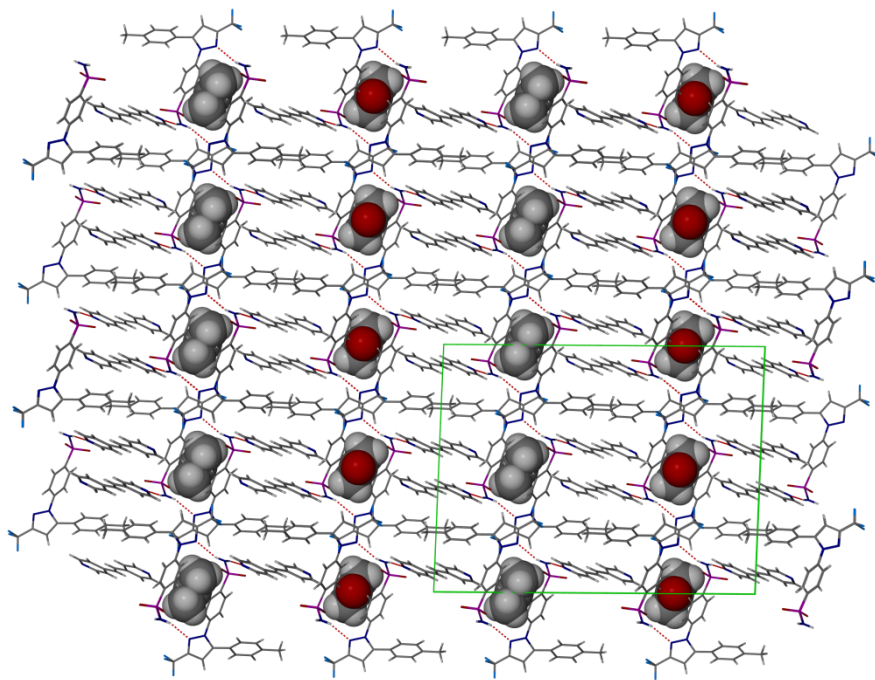
(a)



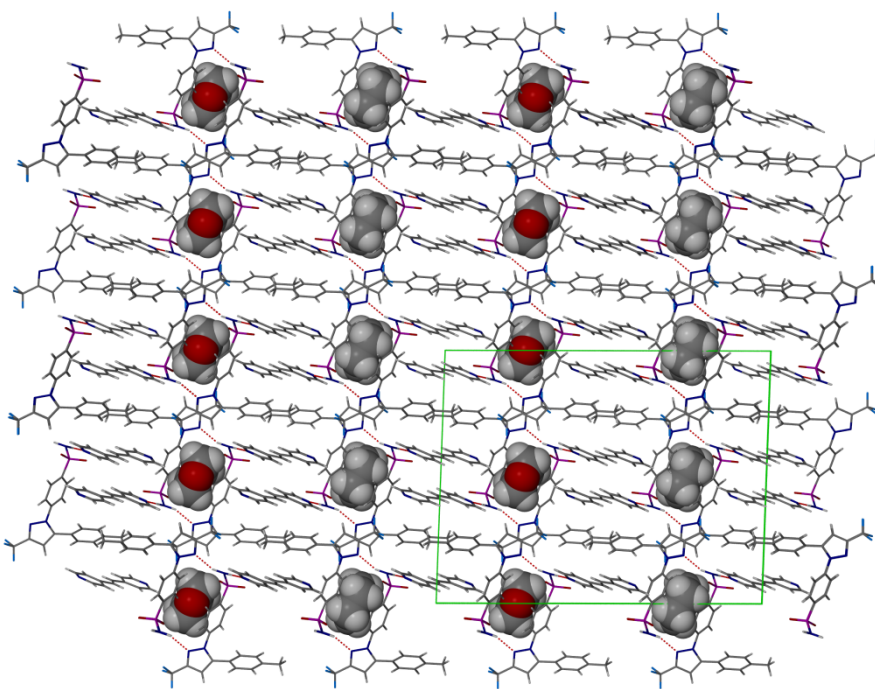
(b)



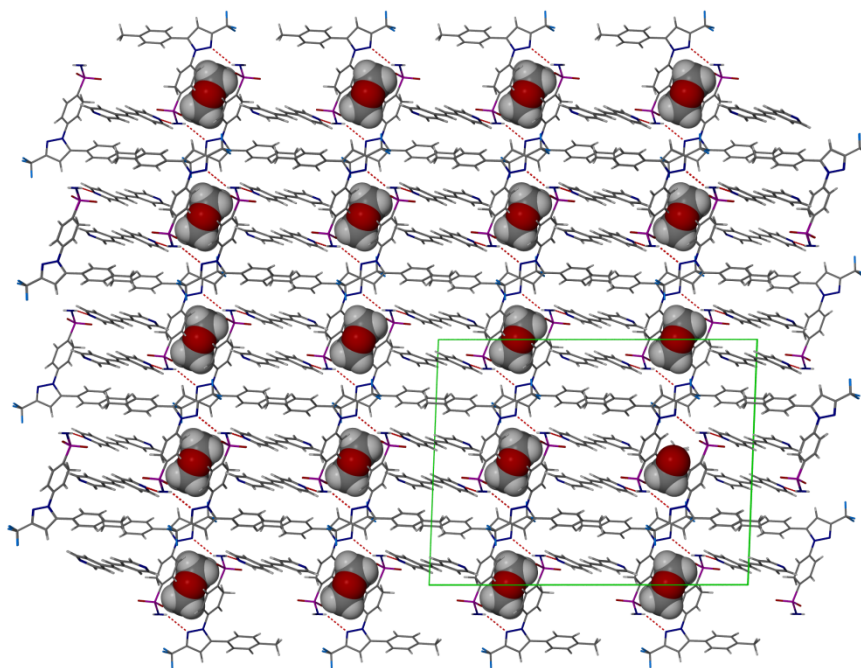
(c)



(d)



(e)



(f)

Fig. S6 Three-dimension packing diagram (view down b-axis) of CEL co-crystal solvates (a) S1a, (b) S1b, (c) S1c, (d) S2a, (e) S2b, (f) S2c.