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Supporting information for article:

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Supporting Informations

Multicomponent solid forms of Lesinurad and cocrystal polymorphs with urea: DFT simulation and solubility study

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Table S1. Hydrogen bond geometry (Å, °)

LES (Form 2)	D-H···A	D-H/ Å	H···A/Å	D···A/Å	D-H···A/°	Symmetry code
	O2–H2···N3	0.82	1.92	2.7214(3)	166	-x,-1/2+y,1/2-z
	C7–H7···N1 (Intra)	0.93	2.57	2.9051(3)	102	--
	C16–H16B···O1	0.97	2.25	3.2088(3)	172	-x,1/2+y,1/2-z
LES-MeOH	O1–H10···O10	0.85	1.81	2.6443(3)	169	-1+x,-1+y,z
	O10–H10O···N3	0.85	1.90	2.7486(3)	172	1-x,-y,-z
	C9–H9···N1 (Intra)	0.95	2.53	2.8707(3)	101	--
	C11–H11···O2	0.89	2.56	3.2381(4)	133	-x,-y,1-z
LES-EtOH	O1–H1···O3	0.82	1.81	2.5985(12)	162	x,-1+y,z
	O3–H3···N2	0.82	1.99	2.8136(13)	178	1/2-x,1/2+y,1/2-z
	C6–H6···N1 (Intra)	0.93	2.56	2.8846(13)	101	--
	C11–H11···N3	0.93	2.53	3.4243(15)	163	1-x,-y,1-z
LES–CAF	O2–H2···N3	0.85	1.81	2.6647(1)	178	-x,1/2+y,1/2-z
	C6–H6···O1	0.95	2.38	3.1972(2)	145	-x,-1/2+y,1/2-z
	C7–H7···N1 (Intra)	0.95	2.55	2.8783(2)	100	--
	C9–H9···N7 (O5)	0.95	2.49	3.4237(2)	168	1-x,-y,1-z
	C16–H16A···O4	0.99	2.33	3.0384(2)	128	--

	C16–H16B···O1	0.99	2.40	3.3671(2)	164	-x,-1/2+y,1/2-z
	C23–H23C···O5 (Intra)	0.98	2.31	2.7626(1)	107	--
	C24–H24A···O4 (Intra)	0.98	2.33	2.7614(1)	106	--
LES–NAM	O2–H2···O3	0.82	1.80	2.5197(3)	145	-x,-1/2+y,1/2-z
	N4–H4A···O1	0.86	2.27	3.0907(3)	160	-x,1/2+y,1/2-z
	N4–H4B···N2	0.86	2.29	3.1317(3)	165	-x,1-y,-z
	C7–H7···N1 (Intra)	0.93	2.61	2.9283(3)	101	--
	C12–H12B···O3	0.97	2.58	3.5024(4)	159	1-x,-1/2+y,1/2-z
	C23–H23···N2	0.93	2.55	3.4727(3)	174	-x,1-y,-z
	C23–H23···N3	0.93	2.44	3.2949(3)	153	-x,1-y,-z
LES–URE (Form I)	O2–H2···O3	0.82	1.78	2.5962(3)	177	1+x,y,z
	N4–H4A···O1	0.86	2.14	2.9518(3)	157	-1+x,y,z
	N4–H4B···N3	0.86	2.50	3.3131(4)	159	1-x,-y,1-z
	N5–H5A···O1	0.86	2.27	3.0486(3)	150	-1+x,y,1+z
	C7–H7···N1 (Intra)	0.93	2.60	2.9243(3)	101	--
	C10–H10···S1	0.93	2.73	3.4504(4)	135	1-x,1-y,1-z
LES–URE (Form II)	O2–H2···O5	0.82	1.80	2.5821(1)	158	1-x,-y,1-z
	O3–H3···O6	0.82	1.72	2.5309(1)	168	-1+x,3/2-y,-1/2+z
	N11–H11A···O6	0.86	2.26	2.9128(1)	133	1-x,-1/2+y,1/2-z
	N11–H11B···N5	0.86	2.36	3.1756(1)	157	1-x,1-y,-z
	N12–H12A···N4	0.86	2.25	3.0940(1)	166	1-x,1-y,-z
	N12–H12B···O1	0.86	2.23	3.0212(1)	153	1-x,-y,1-z
	N13–H13A···N1	0.86	2.46	3.3129(2)	171	1+x,1/2-y,-1/2+z

	N14–H14A···O1	0.86	2.57	2.9598(1)	109	1+x,1/2-y,-1/2+z
	N14–H14A···N2	0.86	2.23	3.0664(1)	166	1+x,1/2-y,-1/2+z
	N14–H14B···O4	0.86	2.13	2.9583(1)	161	1+x,3/2-y,1/2+z
	C11–H11···N3 (Intra)	0.93	2.58	2.8861(1)	100	--
	C17–H17A···N12	0.97	2.59	3.5308(2)	163	1-x,1/2+y,1/2-z
	C23–H23B···N4 (Intra)	0.97	2.59	3.0215(1)	107	--
	C31–H31···N6 (Intra)	0.93	2.50	2.8391(1)	101	--
	C34–H34···O5	0.93	2.57	3.4759(2)	164	1-x,1/2+y,1/2-z

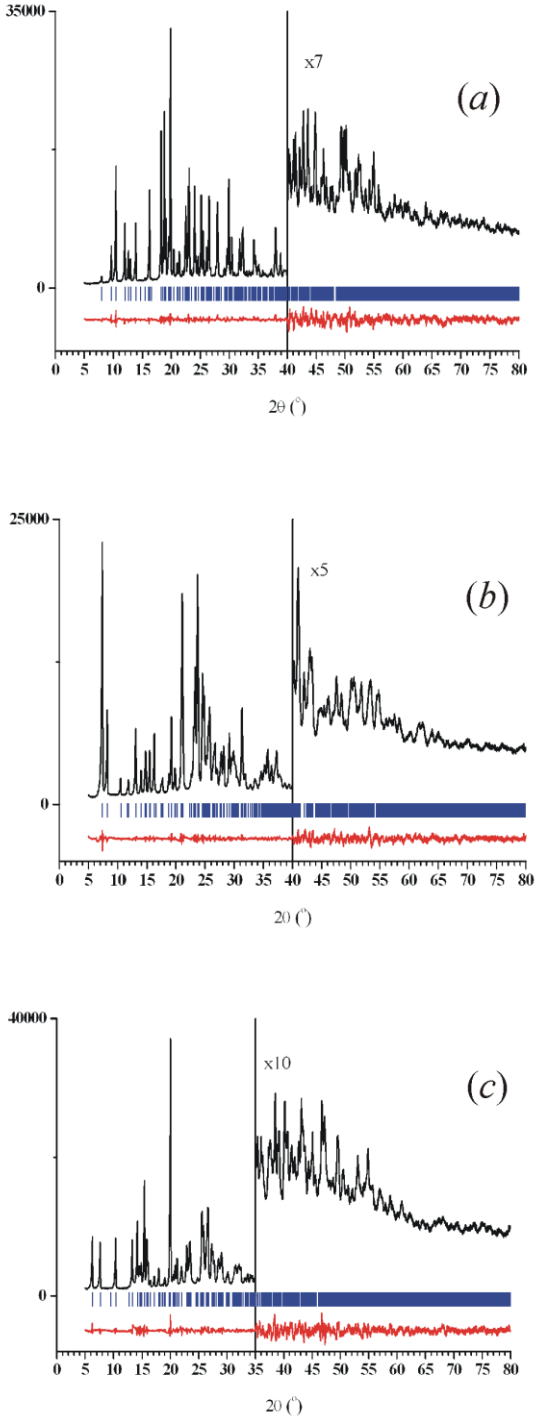


Figure S1. The Rietveld plots for (*a*) LES (Form 2), (*b*) LES–URE (Form I) and (*c*) LES–NAM showing the experimental (black) and difference (experimental minus calculated) curves after the final bond-restrained Rietveld refinements. The vertical blue bars denote calculated positions of the diffraction peaks.

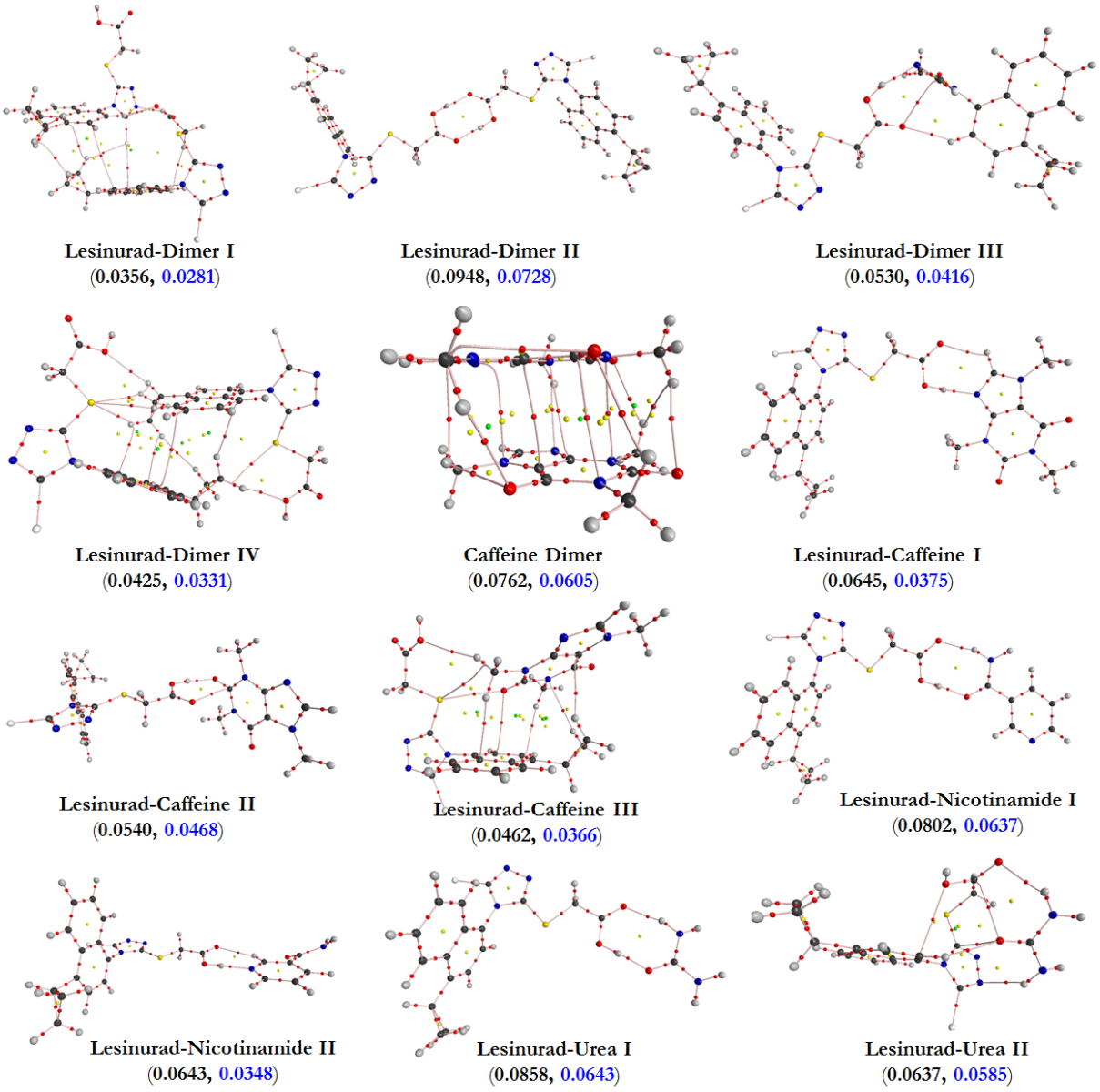


Figure S2. Molecular graphs of various homo and heterosynthons obtained from AIM topography. The calculated total electron density values ($\rho(r_c)$, black) and its Laplacian ($\nabla^2\rho(r_c)$, blue color) at the BCPs shown in parenthesis (in a.u.).

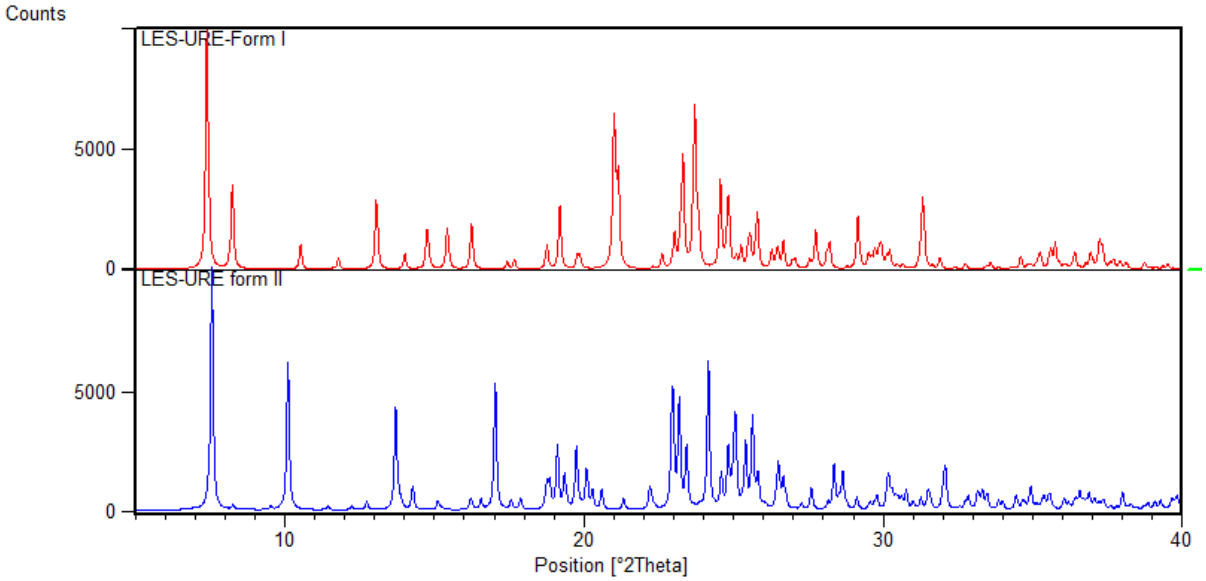
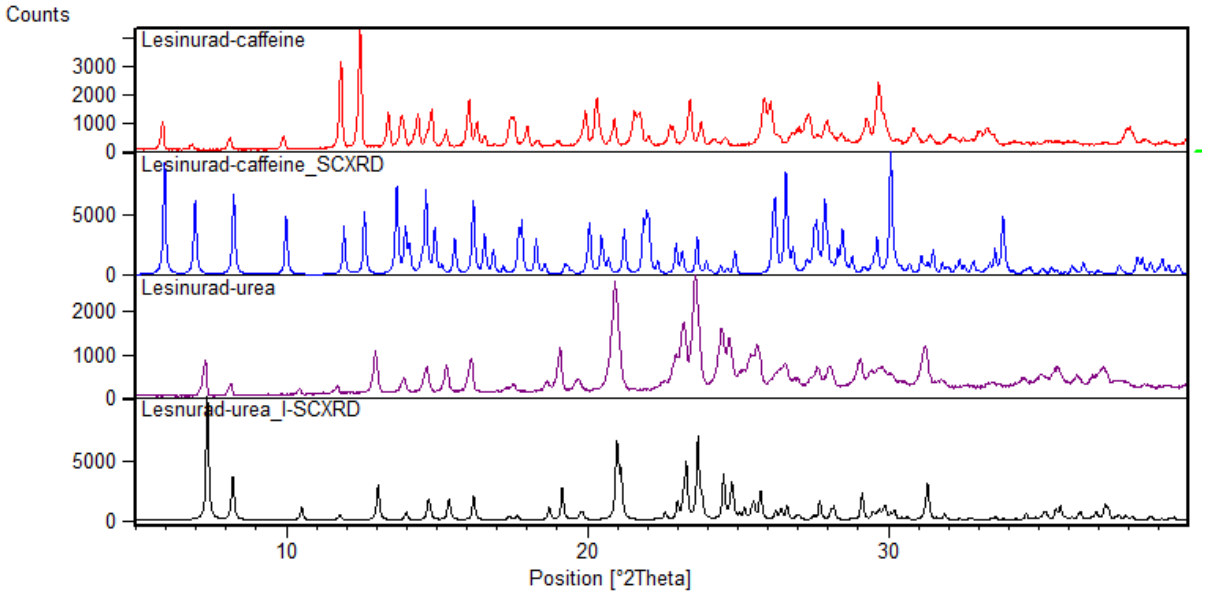
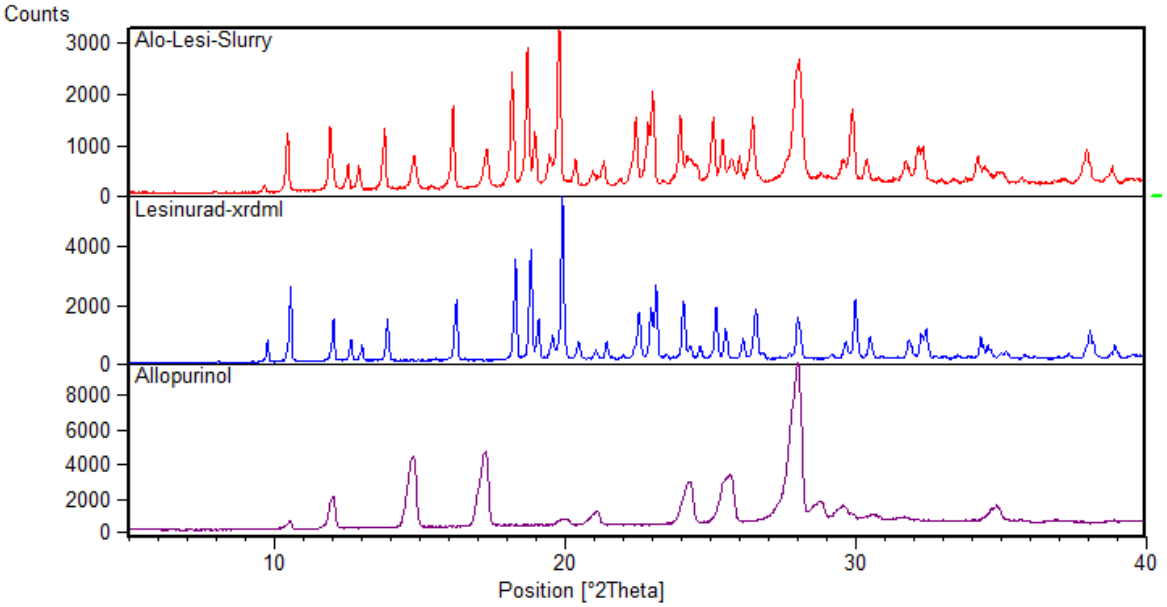


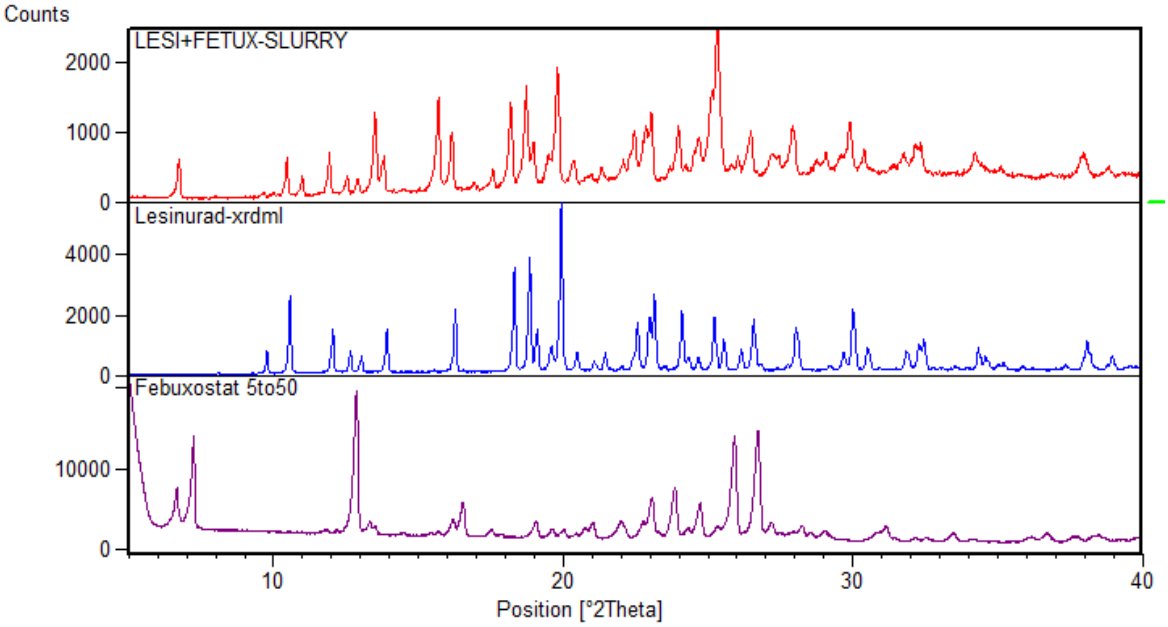
Figure S3. Calculated X-ray patterns of LES-URE cocrystal polymorphs from crystal structures



(a)

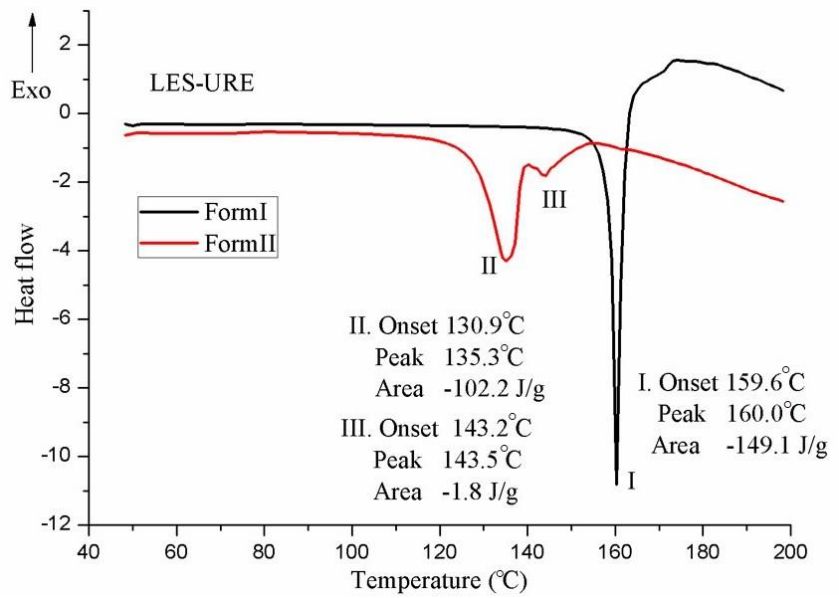


(b)

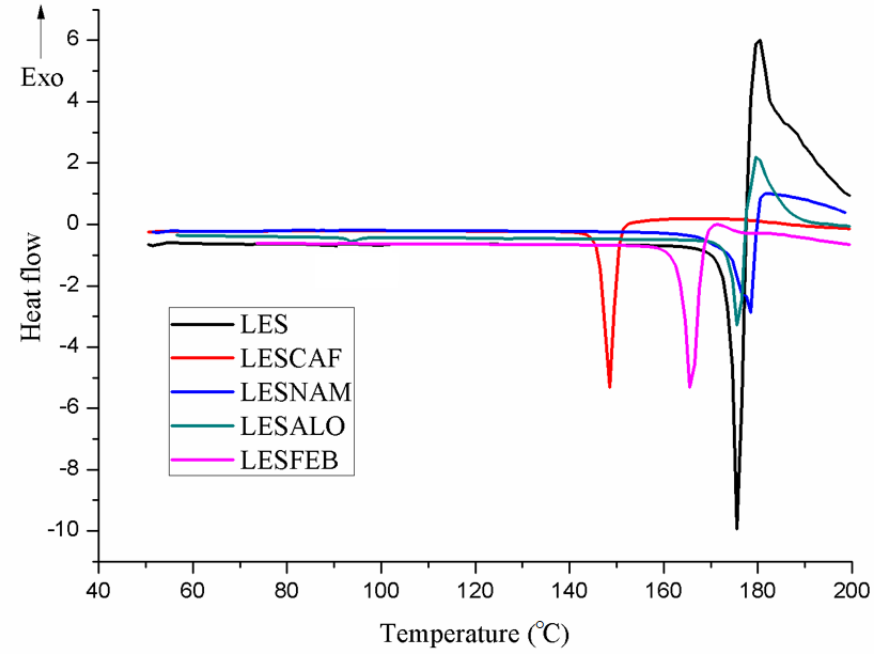


(c)

Figure S4. PXRD comparison of LES-CAF and LES-URE (Form I) with their simulated X-ray patterns, (b) LES-ALO (1:1) (c) LES-FEB (1:1) after slurry experiment with individual components.

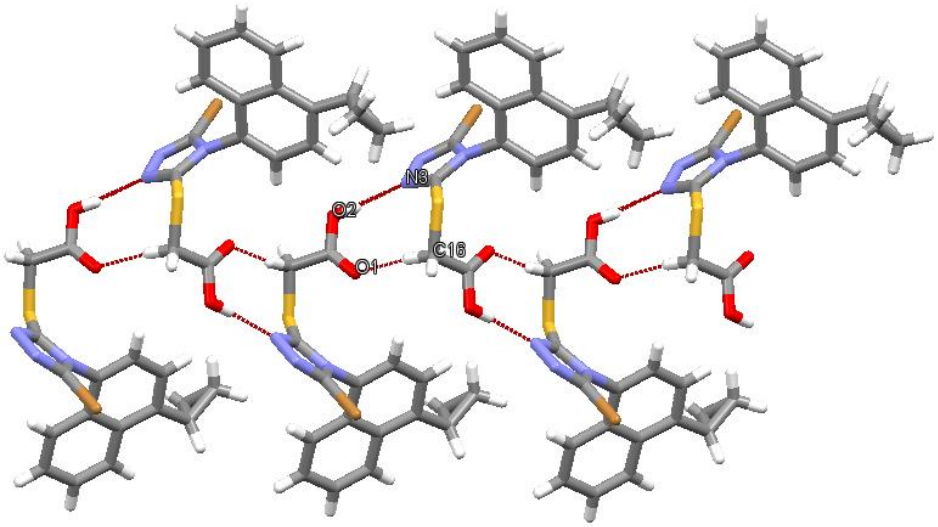


(a)

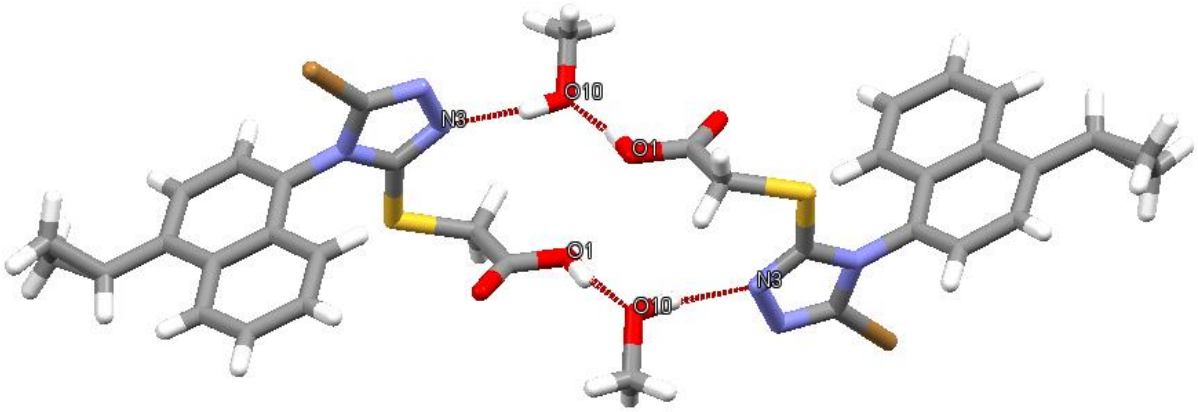


(b)

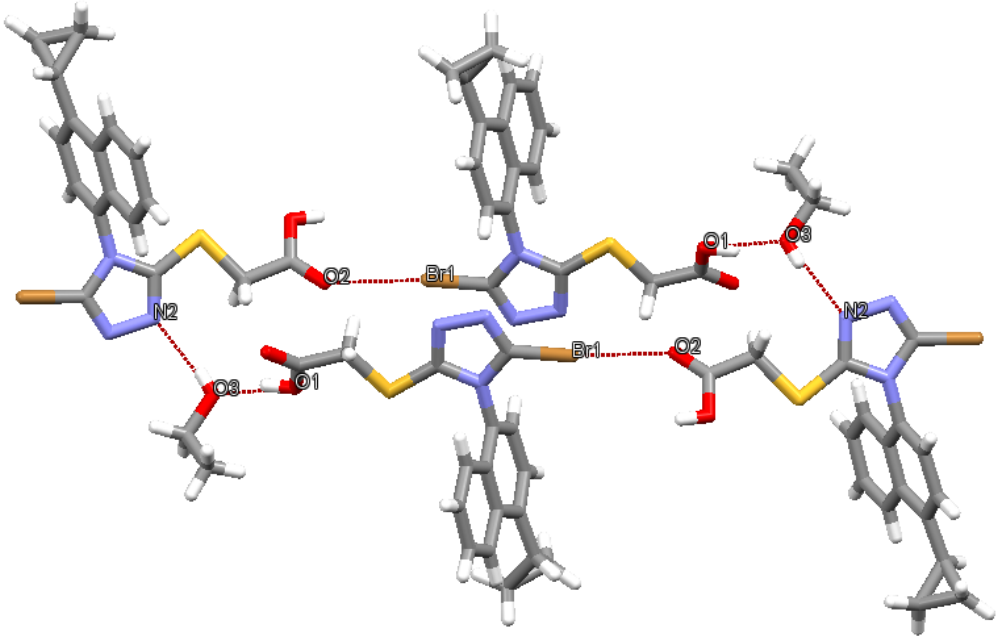
Figure S5. DSC comparison of (a) LES-URE cocrystal polymorphs and (b) other binary systems



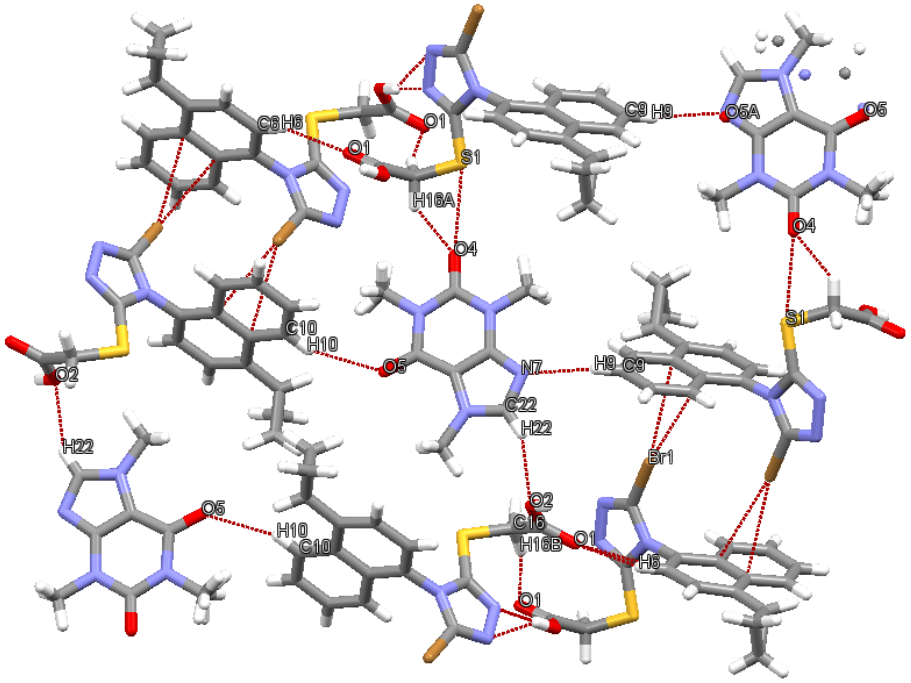
(a)



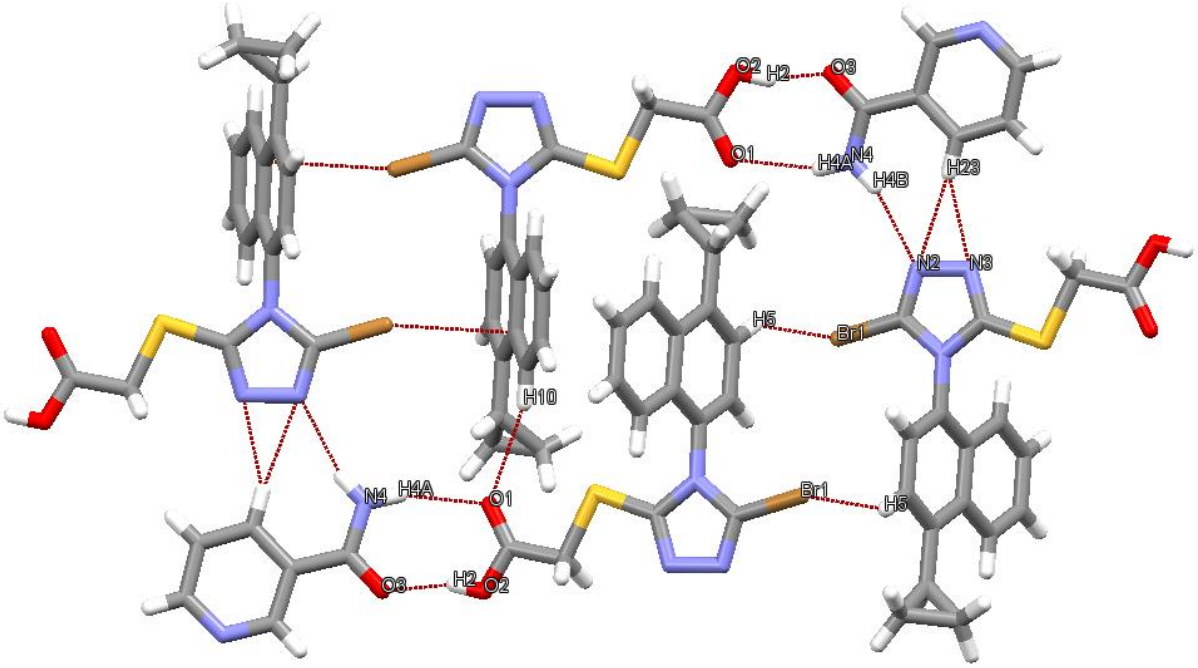
(b)



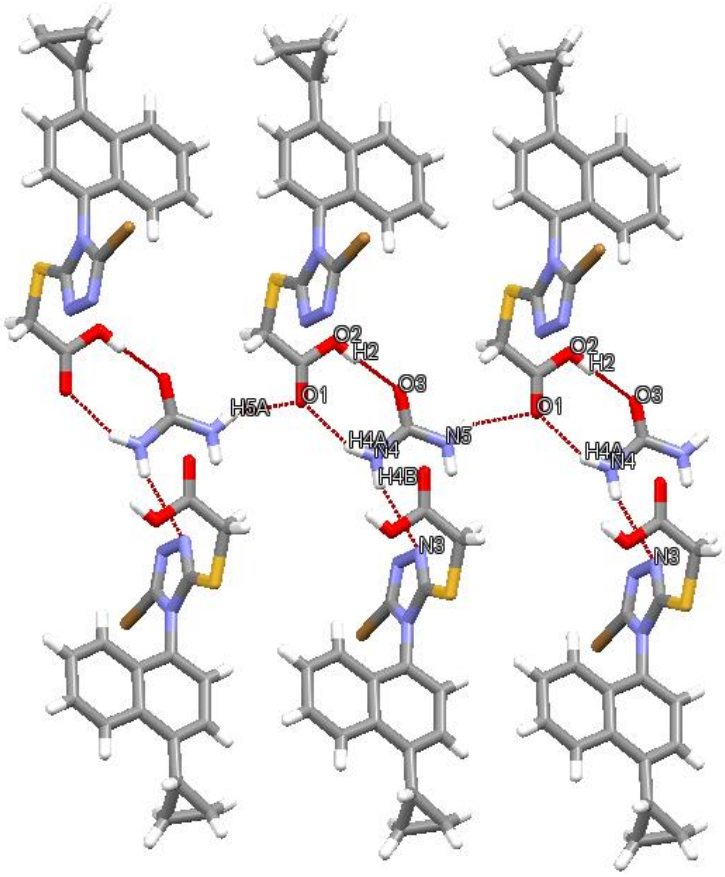
(c)


C8 H8
O1
O1
S1
H16A
C9 H9
O5A
O5
O4
O4
S1
C10
H10
O5
N7
H9 C9
O2
C22
H22
H22
Br1
O5
O2
C16
H16B
O1
H8
C10
H10
O1

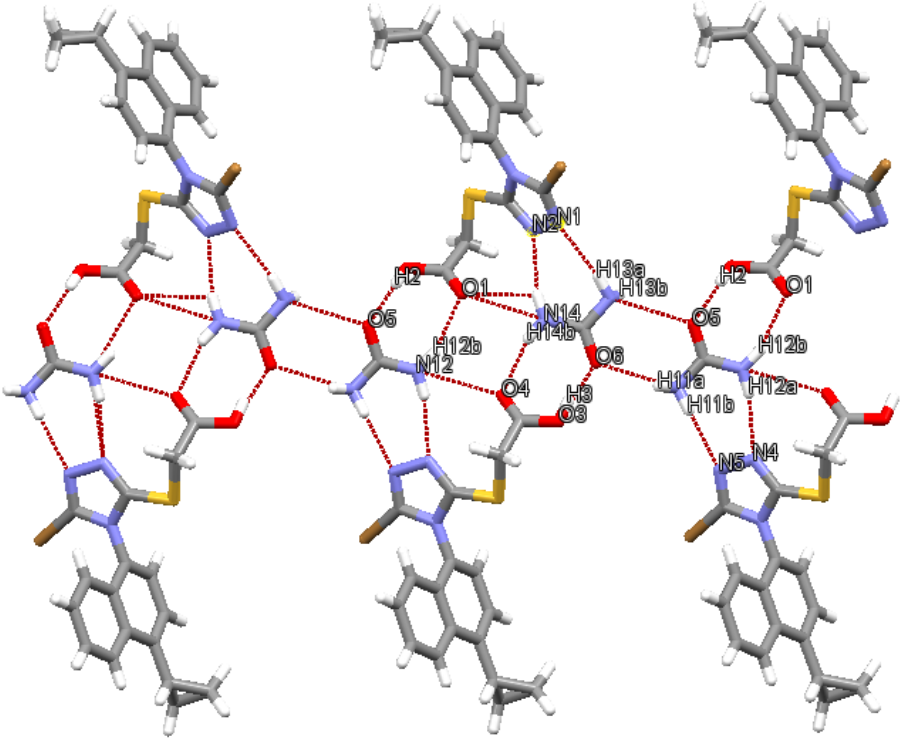
(d)


O2 H2
O3
O1
H4A
N4
H4B
H23
N2
N3
H5
Br1
H10
N4 H4A
O1
Br1
H5
O3
H2
O2

(e)



(f)



(g)

Figure S6. Hydrogen bonding diagram of (a) LES (Form 2), (b) LES-MeOH, (c) LES-EtOH, (d) LES-CAF, (e) LES-NAM, (f) LES-URE (Form I) and (g) LES-URE (Form II).