Co-Crystals of Sulfamethazine with Some Carboxylic Acids and Amides: Co-Former Assisted Tautomerism in an Active Pharmaceutical Ingredient and Hydrogen Bond Competition Study

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Table S1. Geometrical parameters of hydrogen bonds in all the co-crystals.

D—H…A	D…H (Å)	H…A(Å)	D…A (Å)	D—H…A (deg)
Cocrystal SFZ/HBA				
N1 -- H1 .. O3	0.97(3)	1.79(3)	2.756(2)	177.7(16)
O4 -- H4 .. N3	0.79(4)	2.01(4)	2.788(2)	169(5)
N4 -- H4A .. N2	0.91(3)	2.59(3)	3.477(2)	168(2)
N4 -- H4B .. O1	0.90(3)	2.22(3)	3.104(2)	165(3)
O5 -- H5 .. N4	0.73(4)	2.13(4)	2.832(3)	163(4)
C5 -- H6 .. O2	0.9300	2.5900	3.374(2)	142.00
C6 -- H6A .. O5	0.9600	2.5500	3.487(3)	166.00
C18 -- H18 .. O1	0.9300	2.5700	3.347(2)	142.00
Cocrystal SFZ/DHB				
N3 -- H3 .. O4	0.89(3)	1.90(3)	2.791(2)	176(3)
N4 -- H4B .. O1	0.90(3)	2.31(3)	3.178(2)	162(2)
O5 -- H5A .. O4	0.99(4)	1.68(5)	2.586(2)	151(4)
O3 -- H5B .. N2	0.88(3)	1.82(3)	2.696(2)	174(3)
O6 -- H7 .. N4	0.81(4)	2.17(4)	2.919(2)	154(3)
C1 -- H1C .. O6	0.9600	2.5100	3.444(3)	166.00
C18 -- H18 .. O1	0.9300	2.5500	3.335(2)	142.00
Cocrystal SFZ/DCB				
O1 -- H1 .. N4	0.72(4)	1.96(4)	2.679(3)	174(4)
N2 -- H2 .. O2	0.80(3)	2.04(3)	2.839(3)	178(2)
N3 -- H3A .. O3	0.85(3)	2.51(3)	3.223(4)	143(3)
N3 -- H3B .. O4	0.90(4)	2.38(4)	3.192(3)	150(3)
C3 -- H3 .. O1	0.9300	2.3900	2.709(3)	100.00
Cocrystal SFZ/SOR				
N2 -- H2 .. O3	0.83(3)	2.01(3)	2.830(2)	176(2)
O4 -- H4 .. N3	0.91(3)	1.79(3)	2.694(2)	177(4)
N4 -- H4A .. O1	0.85(4)	2.29(4)	2.953(4)	135(4)
N4 -- H5A .. O3	0.92(4)	2.29(4)	3.182(4)	164(3)

C9 -- H9 .. O2	0.9300	2.4800	2.874(3)	105.00
C17 -- H17 .. O4	0.9300	2.4800	2.790(2)	100.00
Cocrystal SFZ/FUM/ACN				
N3 -- H3 .. O4	0.88(2)	1.91(2)	2.7866(16)	173.1(19)
N4 -- H4A .. O3	0.90(2)	2.14(2)	3.0137(18)	164.6(19)
N4 -- H4B .. O2	0.86(2)	2.20(2)	3.0072(18)	156.1(17)
O5 -- H5A .. N1	0.92(2)	1.78(2)	2.6926(16)	172(2)
C5 -- H5 .. O2	0.9300	2.5400	2.8954(17)	103.00
C6 -- H6 .. N5	0.9300	2.5800	3.270(7)	131.00
Cocrystal SFZ/1HNA				
O2 -- H2 .. N4	1.04(3)	1.57(3)	2.6000(17)	172(2)
N2 -- H2C .. O1	0.91(2)	1.97(2)	2.8770(18)	176.4(19)
O3 -- H3 .. O1	0.88(2)	1.82(2)	2.6016(16)	148(2)
N3 -- H3A .. O6	0.88(2)	2.07(2)	2.949(2)	173.1(19)
N3 -- H3B .. O3	0.88(2)	2.18(2)	3.0451(18)	169.6(18)
N5 -- H5A .. O10	0.88(2)	2.17(2)	3.0399(18)	168(2)
N5 -- H5B .. O4	0.87(2)	2.13(2)	2.9872(19)	168(2)
N6 -- H6 .. O8	0.85(2)	2.06(2)	2.9006(18)	173(2)
O9 -- H9 .. N8	1.05(3)	1.56(3)	2.6001(17)	171(2)
O10 -- H10 .. O8	0.94(2)	1.77(2)	2.6034(16)	147(2)
C11 -- H11 .. O2	0.9300	2.4200	2.740(2)	100.00
C16 -- H16 .. O4	0.9300	2.5200	2.9044(18)	105.00
C32 -- H32 .. O6	0.9300	2.5500	2.9183(18)	104.00
C46 -- H46 .. O9	0.9300	2.4300	2.742(2)	100.00
Cocrystal SFZ/BEN				
N2 -- H2 .. O3	0.79(5)	1.93(5)	2.704(5)	166(6)
N4 -- H4A .. O1	0.80(8)	2.25(8)	2.950(6)	147(7)
N4 -- H4B .. O2	0.82(5)	2.11(5)	2.924(6)	171(5)
N5 -- H7A .. O1	0.92(5)	2.33(5)	3.168(5)	152(5)
N5 -- H7B .. N3	0.77(6)	2.49(6)	3.235(6)	166(5)
C8 -- H8 .. O2	0.9300	2.5500	2.910(5)	103.00
C14 -- H14 .. O3	0.9300	2.4300	2.748(6)	100.00

Cocrystal SFZ/PIC

N1 -- H1 .. O3	0.97(4)	1.79(3)	2.762(3)	174(3)
N4 -- H4A .. O2	0.86(3)	2.21(3)	3.020(4)	159(3)
N4 -- H4B .. O1	0.91(4)	2.31(4)	3.186(4)	161(3)
N6 -- H7A .. N5	0.96(4)	2.25(3)	2.666(4)	105(2)
N6 -- H7B .. N3	0.85(4)	2.15(4)	2.988(4)	169(4)
C6 -- H6B .. O1	0.9600	2.5300	3.427(4)	156.00

Cocrystal SFZ/HBEN-Triclinic Form

N2 -- H2 .. O4	0.91(4)	1.82(4)	2.722(3)	170(4)
N4 -- H4A .. O1	0.87(4)	2.03(4)	2.867(4)	164(4)
N4 -- H4B .. O3	0.93(9)	2.10(9)	2.885(3)	142(7)
N5 -- H7A .. N3	0.86(4)	2.18(4)	3.032(3)	173(4)
N5 -- H7B .. O2	0.89(4)	2.16(4)	2.995(4)	156(3)
C8 -- H8 .. O1	0.9300	2.4400	2.841(4)	106.00
C15 -- H15 .. O4	0.9300	2.4500	2.768(4)	100.00
C19 -- H19 .. O2	0.9300	2.6000	3.494(4)	162.00

Cocrystal SFZ/HBEN-Monoclinic Form

N1 -- H1A .. N9	0.94(3)	2.20(3)	3.124(3)	168(3)
N2 -- H2 .. O7	0.96(3)	1.75(3)	2.709(2)	173(3)
O2 -- H2B .. O8	0.79(3)	2.01(3)	2.765(3)	160(3)
N13 -- H4A .. O6	0.87(3)	2.28(3)	3.100(3)	157(3)
N13 -- H4B .. N4	0.94(3)	2.15(3)	3.078(3)	168(3)
N5 -- H5A .. O4	0.88(3)	2.02(3)	2.891(3)	168(3)
N5 -- H5B .. O6	0.86(3)	2.17(3)	2.938(3)	149(3)
O8 -- H8 .. N5	0.87(3)	1.88(3)	2.748(3)	172(3)
N11 -- H11A .. O1	0.91(3)	1.78(3)	2.684(2)	173(3)
N12 -- H12A .. O5	0.87(3)	1.97(3)	2.842(3)	175(3)
N12 -- H12B .. O3	0.91(4)	2.19(4)	2.969(3)	144(3)
C5 -- H5 .. O3	0.9300	2.5600	3.486(3)	175.00
C20 -- H20 .. O4	0.9300	2.5400	2.891(3)	103.00
C32 -- H32 .. O5	0.9300	2.4600	2.852(3)	105.00

C35 -- H35 .. O5	0.9300	2.5500	3.286(3)	137.00
C38 -- H38 .. O7	0.9300	2.4400	2.755(3)	100.00
Cocrystal SFZ/3HNA				
N1 -- H1A .. O2	0.84(2)	2.22(2)	3.0416(19)	167(2)
N1 -- H1B .. O5	0.91(3)	2.10(2)	3.0010(19)	171(2)
N4 -- H4 .. O3	0.81(2)	1.94(2)	2.7486(18)	176.8(14)
O4 -- H4A .. N2	0.94(3)	1.71(3)	2.6458(17)	175(3)
O5 -- H5 .. O3	0.87(3)	1.78(3)	2.5869(17)	154(2)
C9 -- H9 .. O1	0.9300	2.4800	2.8643(19)	105.00
C18 -- H18 .. O1	0.9300	2.6000	3.2931(19)	132.00
C20 -- H20 .. O2	0.9300	2.5300	3.305(2)	141.00
C23 -- H23 .. O4	0.9300	2.4100	2.7375(19)	100.00

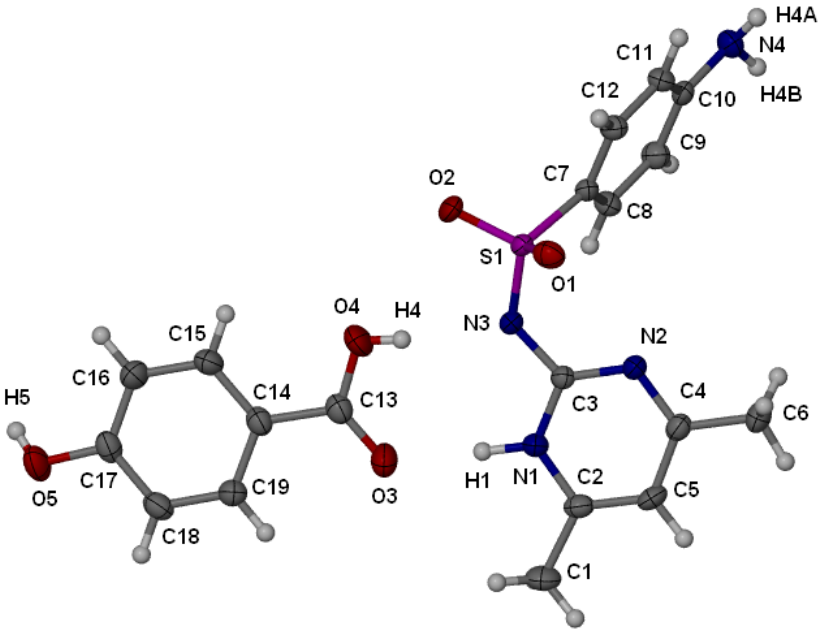

Figure S1. ORTEP diagram of the structure, sulfamethazine SFZ/HBA co-crystal. Displacement ellipsoids are drawn at the 50% probability level.

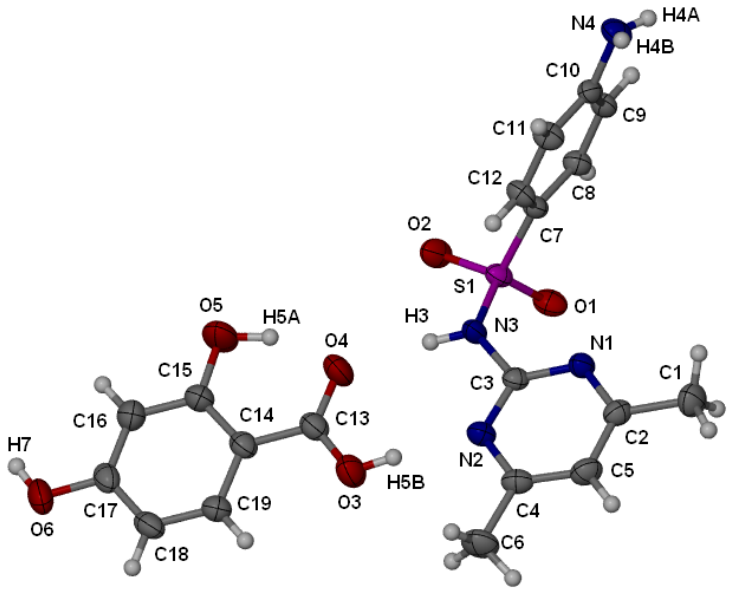

Figure S2. ORTEP diagram of the structure, sulfamethazine SFZ/DHB co-crystal. Displacement ellipsoids are drawn at the 50% probability level.

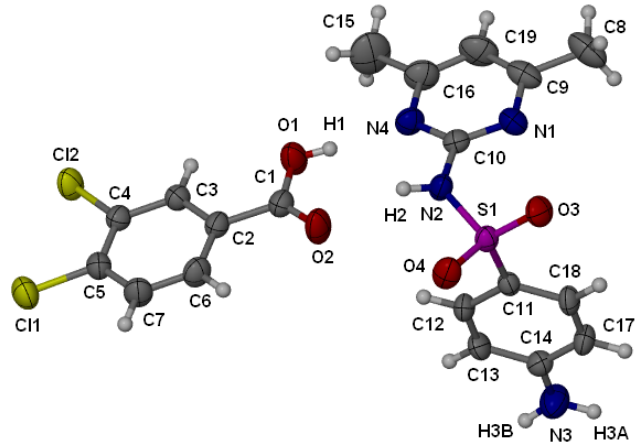

Figure S3. ORTEP diagram of the structure, sulfamethazine SFZ/DCB co-crystal. Displacement ellipsoids are drawn at the 50% probability level.

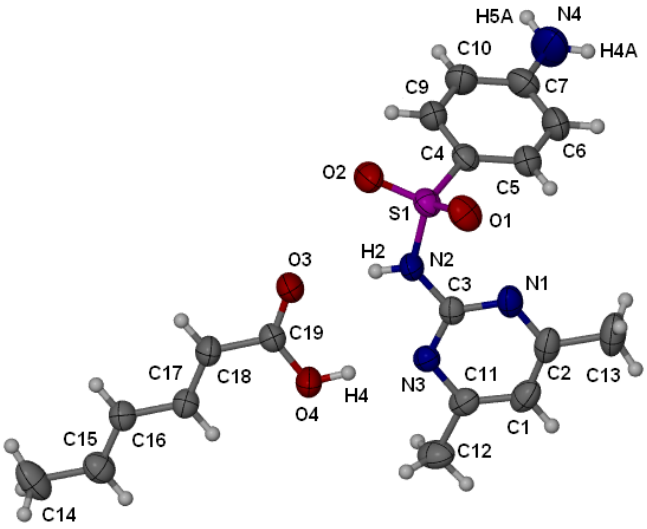

Figure S4. ORTEP diagram of the structure, sulfamethazine SFZ/SOR co-crystal. Displacement ellipsoids are drawn at the 50% probability level.

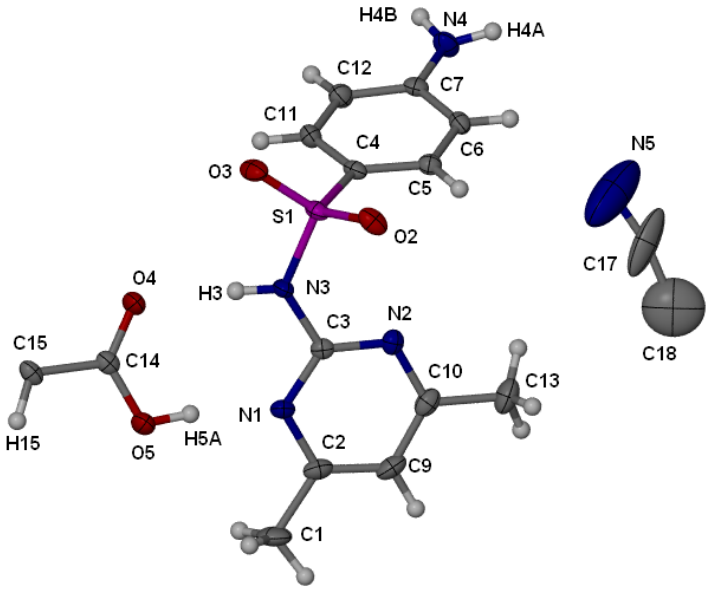

Figure S5. ORTEP diagram of the structure, sulfamethazine SFZ/FUM/ACN (2:1:1) co-crystal solvate. Displacement ellipsoids are drawn at the 50% probability level.

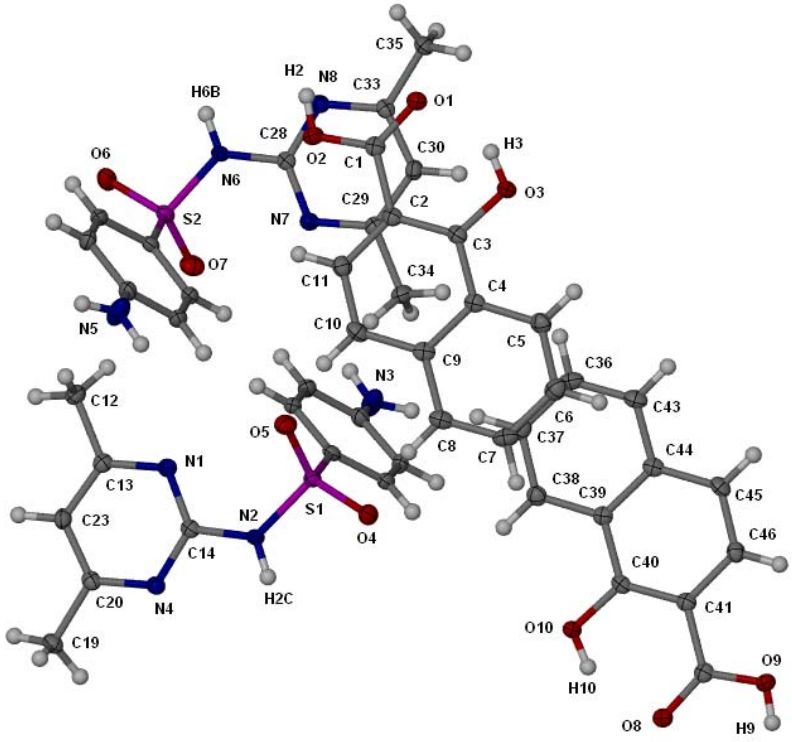

Figure S6. ORTEP diagram of the structure, sulfamethazine SFZ/1HNA co-crystal. Displacement ellipsoids are drawn at the 50% probability level.

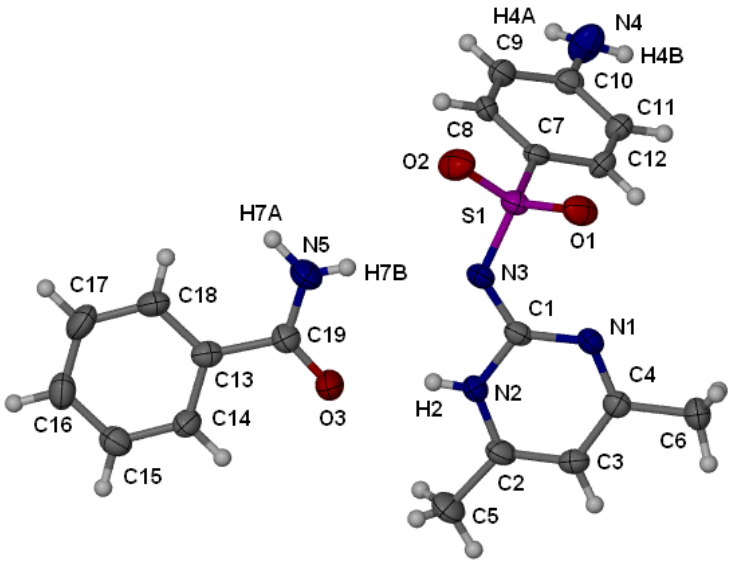

Figure S7. ORTEP diagram of the structure, sulfamethazine SFZ/BEN co-crystal. Displacement ellipsoids are drawn at the 50% probability level.

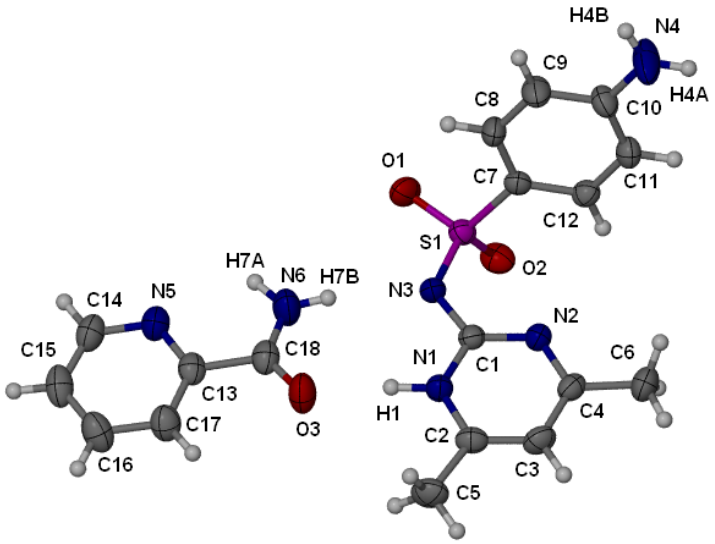

Figure S8. ORTEP diagram of the structure, sulfamethazine SFZ/PIC co-crystal. Displacement ellipsoids are drawn at the 50% probability level.

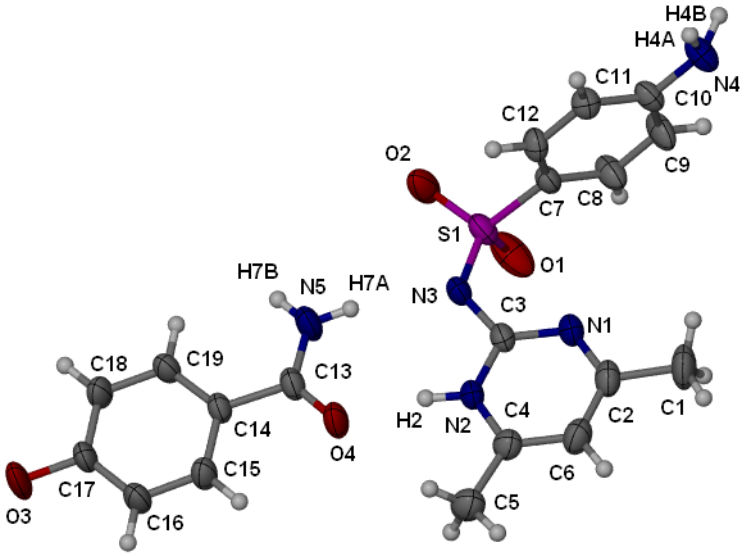

Figure S9. ORTEP diagram of the structure, sulfamethazine SFZ/HBEN (Triclinic) co-crystal.

Displacement ellipsoids are drawn at the 50% probability level.

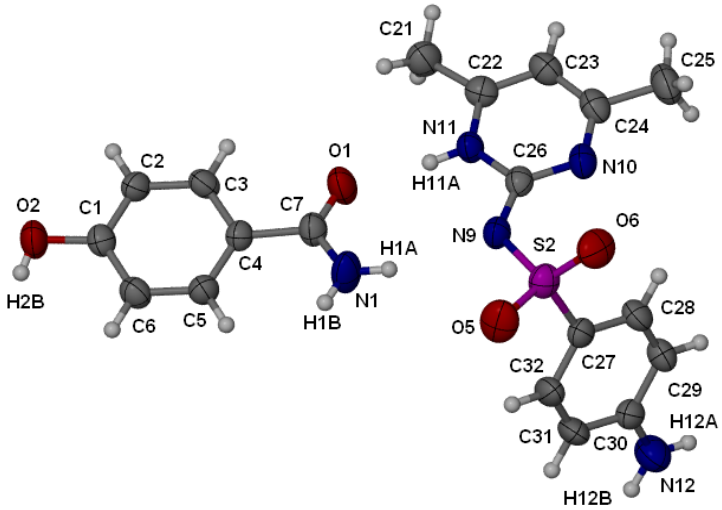

Figure S10. ORTEP diagram of the structure, sulfamethazine SFZ/HBEN (monoclinic) co-crystal.

Displacement ellipsoids are drawn at the 50% probability level.

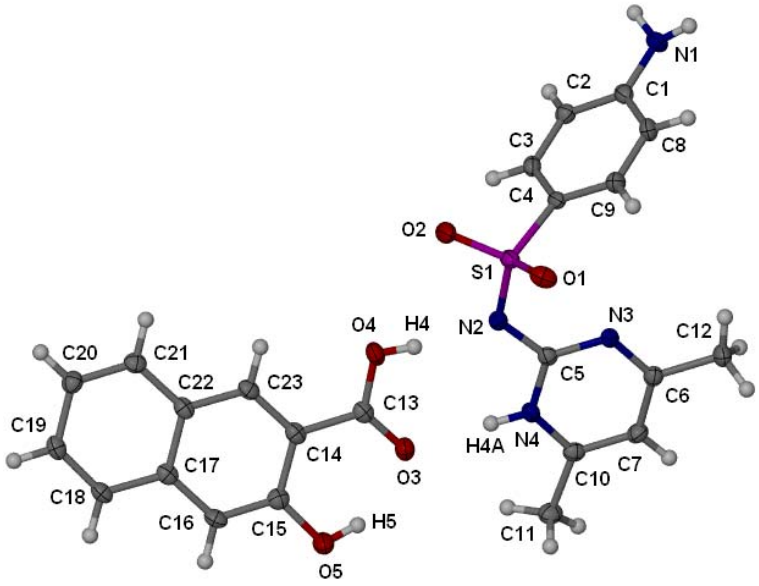

Figure S11. ORTEP diagram of the structure, sulfamethazine SFZ/3HNA co-crystal. Displacement ellipsoids are drawn at the 50 % probability level.

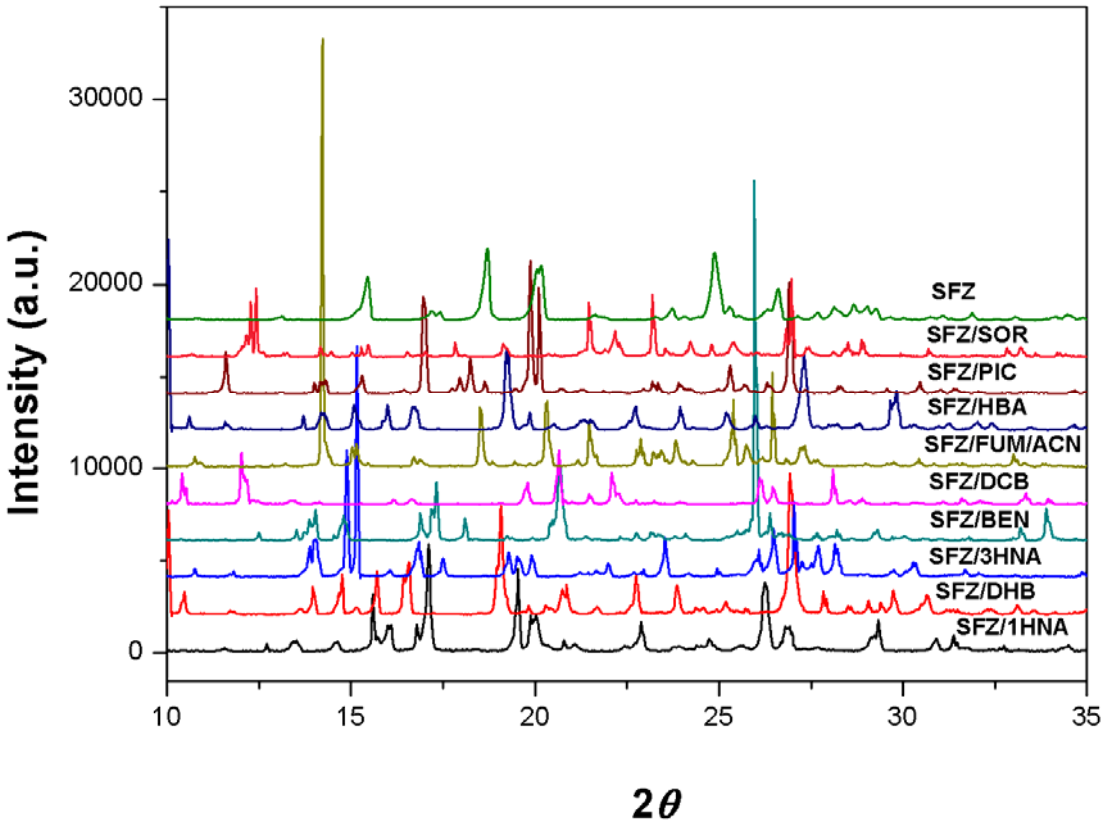

Figure S11. Powder XRD patterns of all the SFZ co-crystals, except SFZ/HBEN polymorphs.

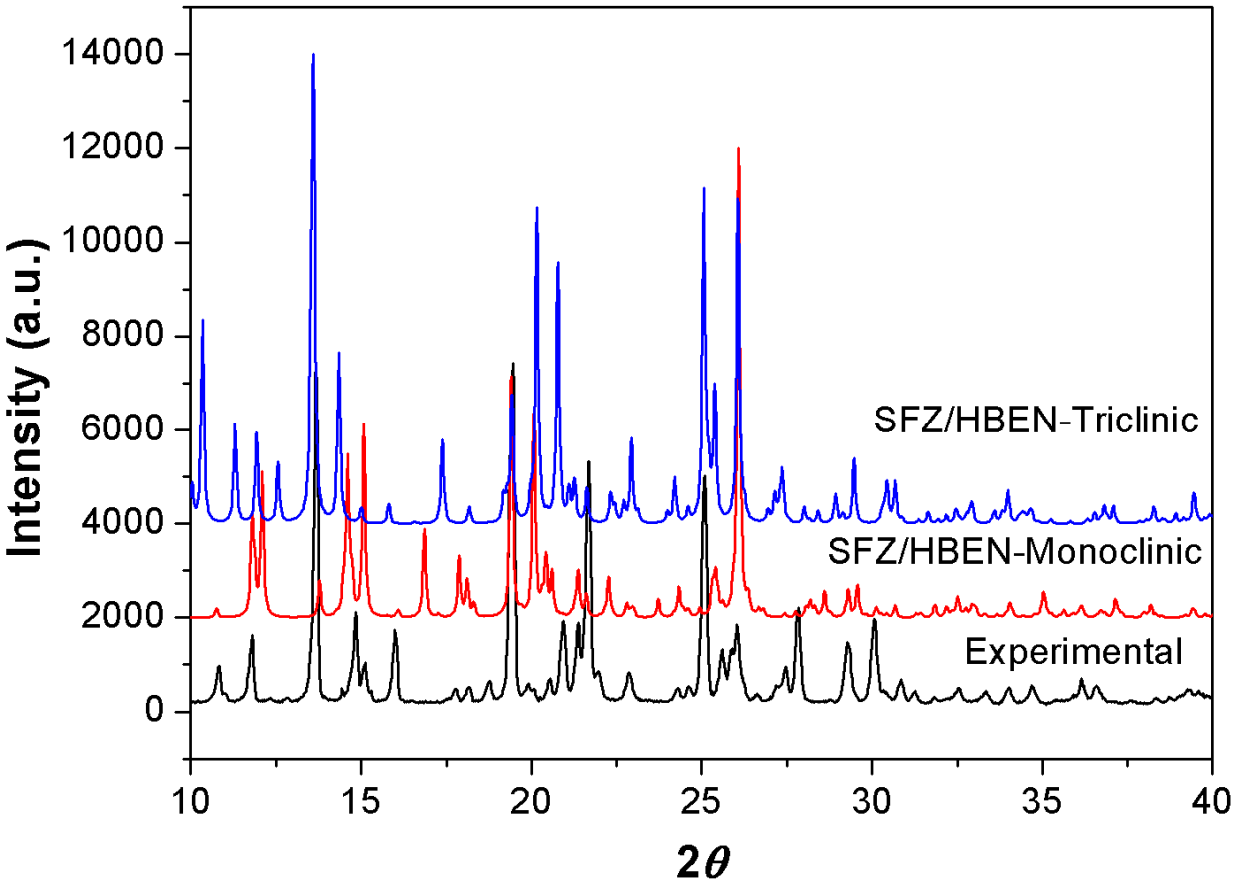

Figure S12. Powder XRD pattern of the mixture of concomitant forms, SFZ/HBEN-T and SFZ/HBEN-M along with their simulated PXRD patterns.

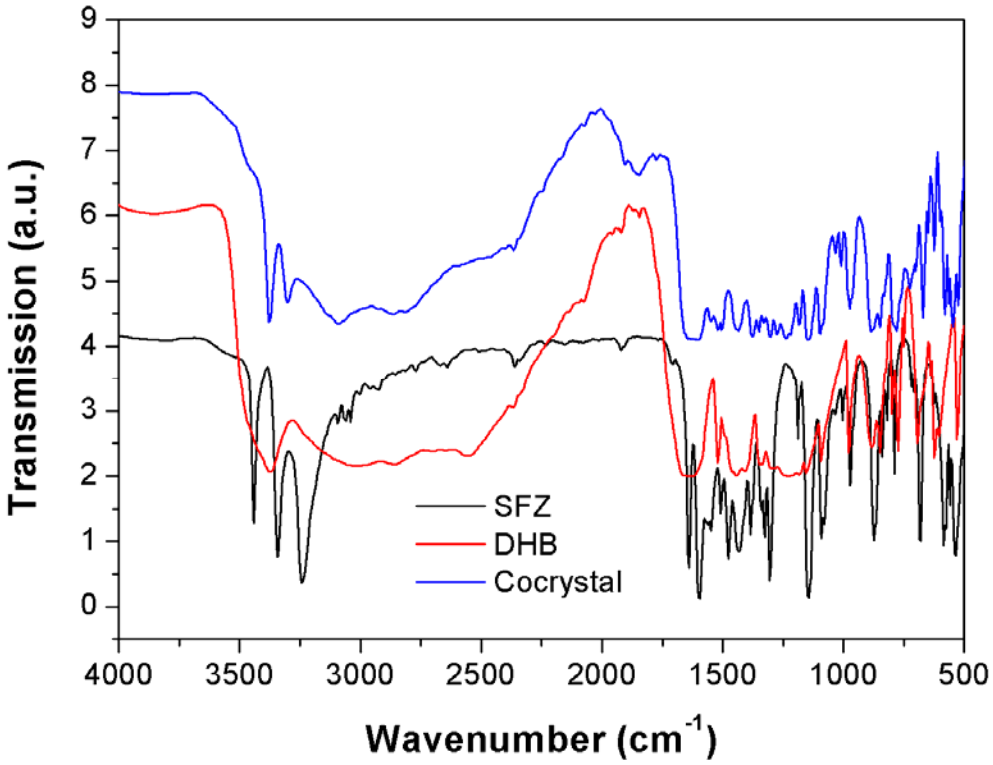

Figure S13. Infrared spectra of the SFZ/DHB co-crystal and the single component co-formers.

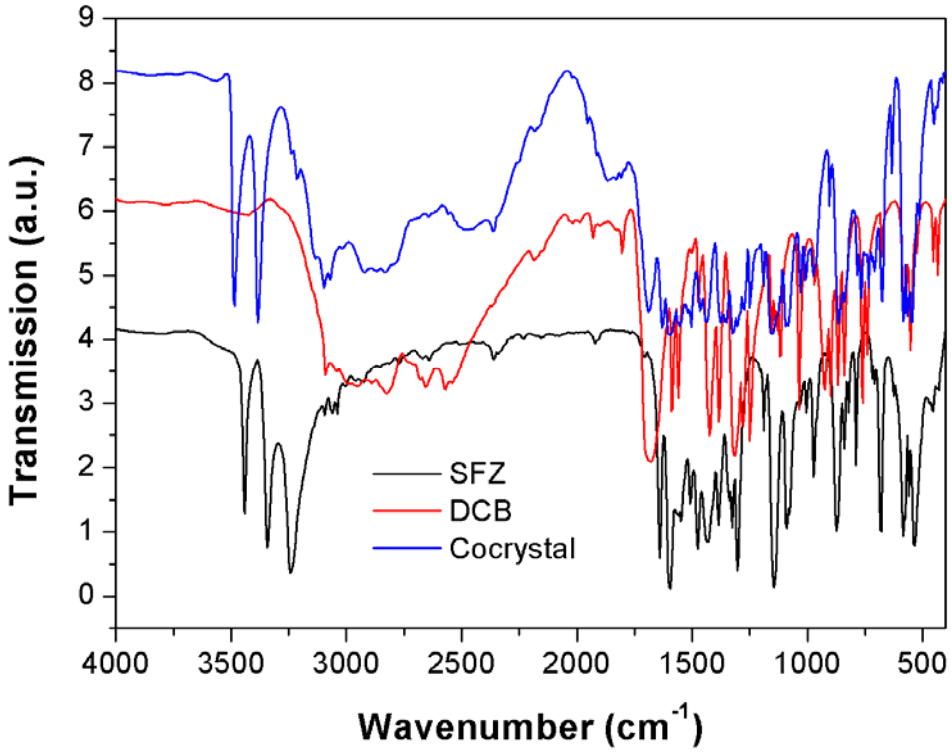

Figure S14. Infrared spectra of the SFZ/DCB co-crystal and the single component co-formers.

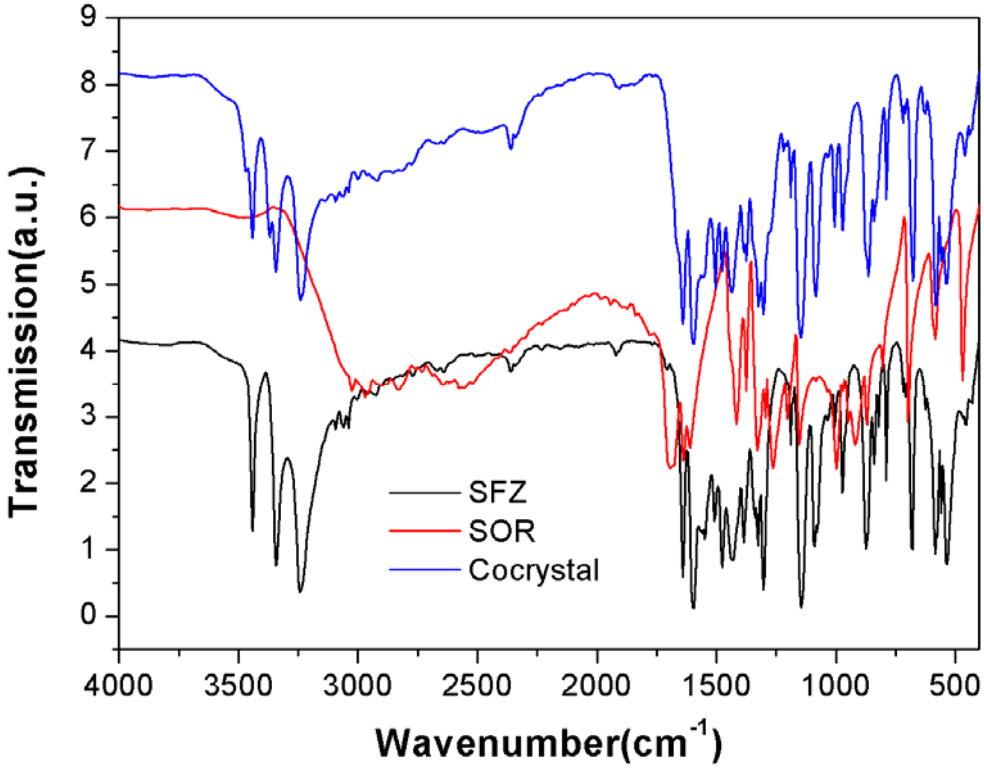

Figure S15. Infrared spectra of the SFZ/SOR co-crystal and the single component co-formers.

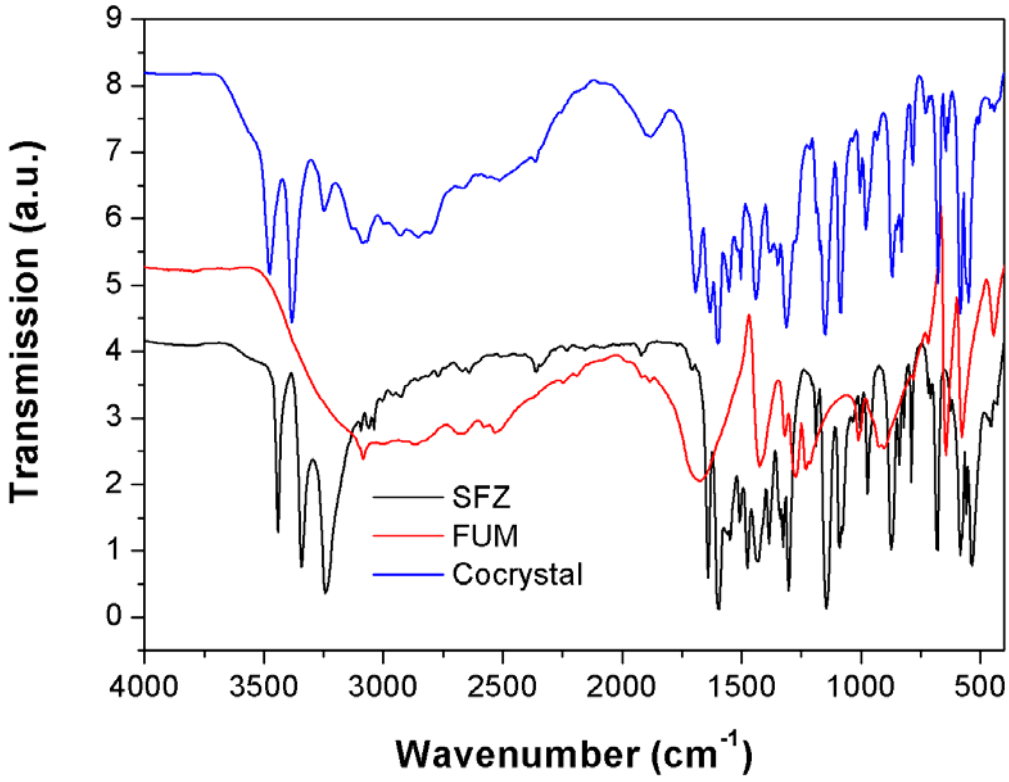

Figure S16. Infrared spectra of the SFZ/FUM/ACN co-crystal solvate and the single component co-formers.

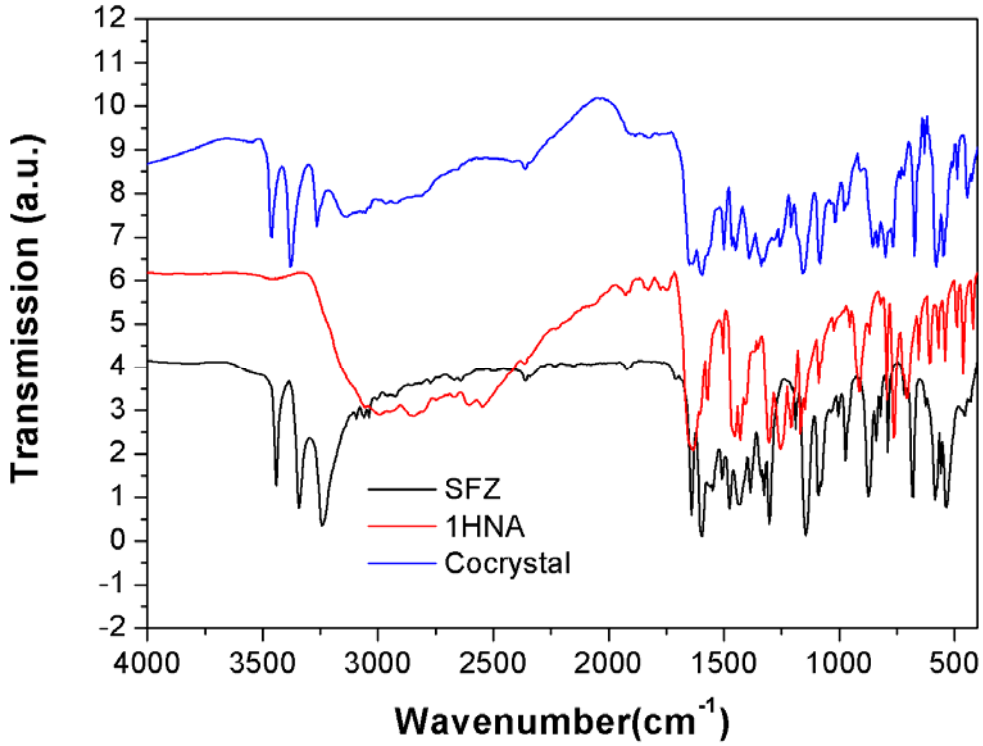

Figure S17. Infrared spectra of the SFZ/1HNA co-crystal and the single component co-formers.

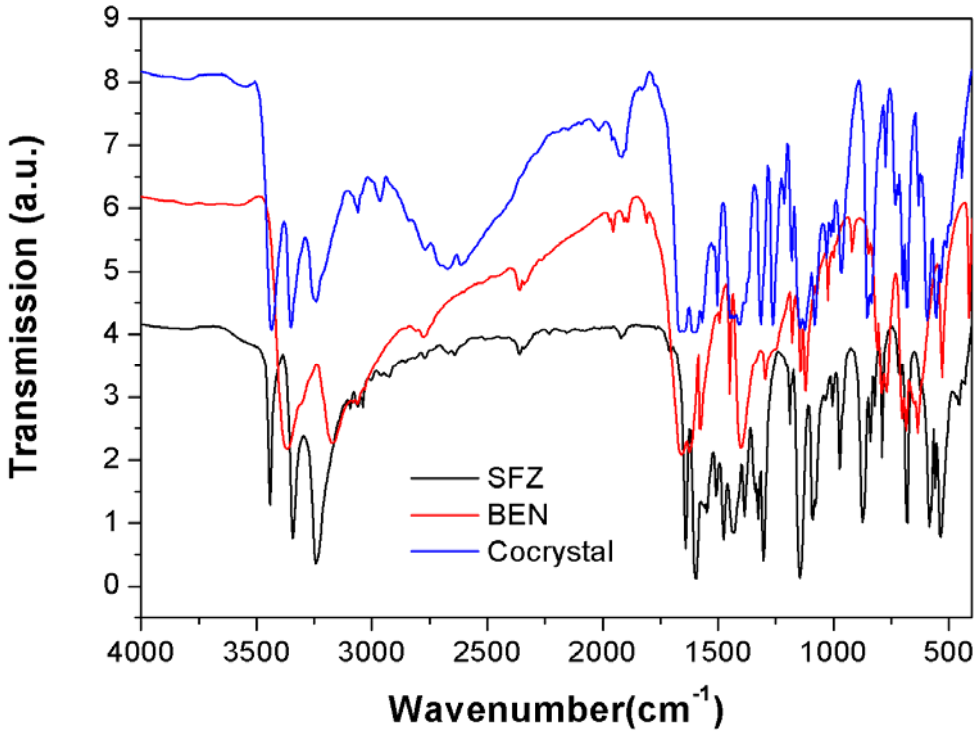

Figure S18. Infrared spectra of the SFZ/BEN co-crystal and the single component co-formers.

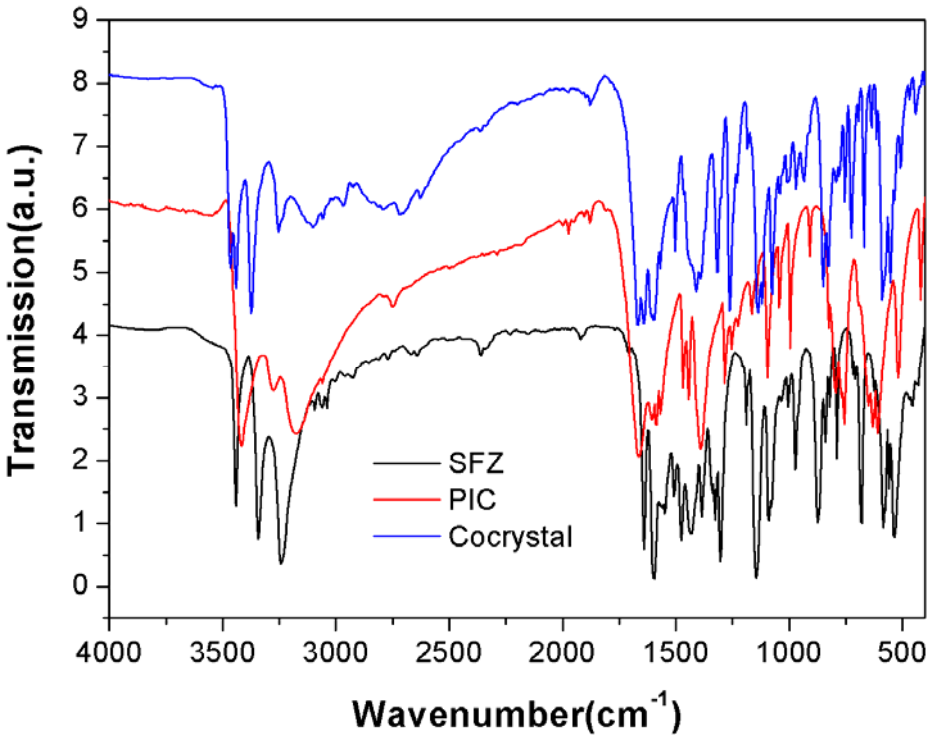

Figure S19. Infrared spectra of the SFZ/PIC co-crystal and the single component co-formers.

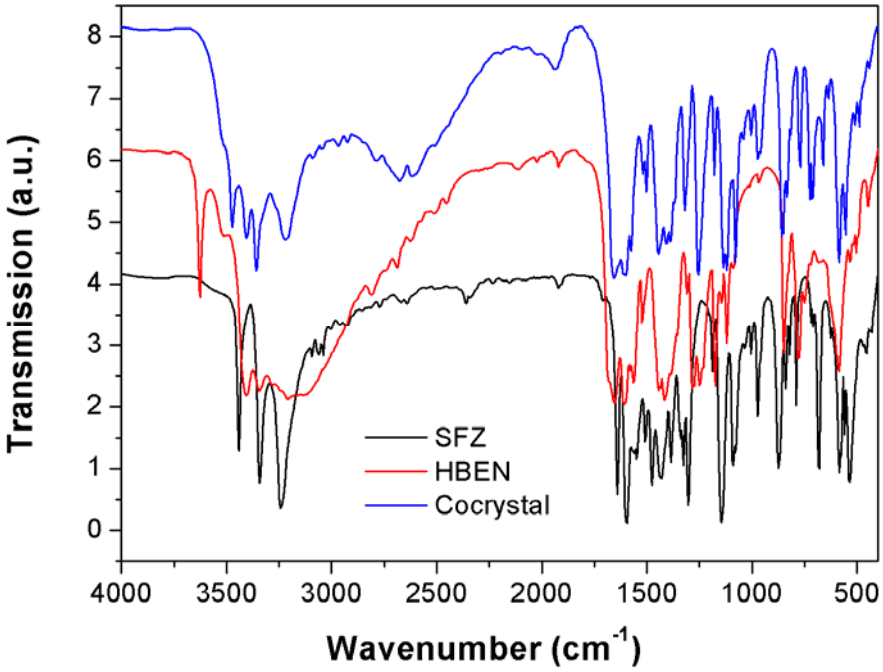

Figure S20. Infrared spectra of the SFZ/HBEN co-crystal (mixture of both the triclinic and monoclinc forms) and the single component co-formers.

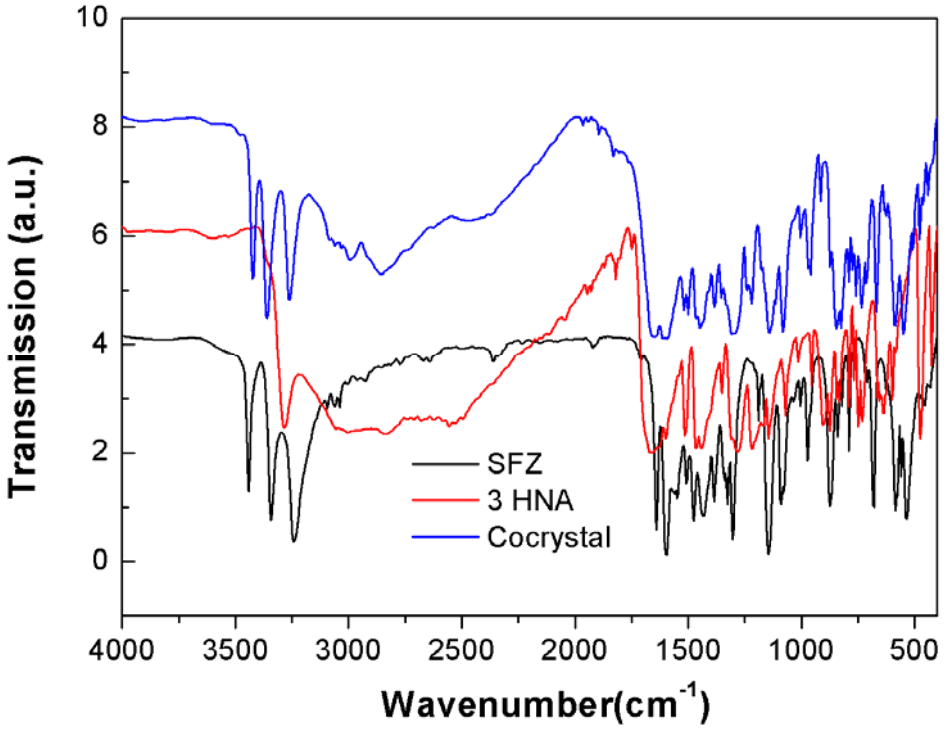

Figure S21. Infrared spectra of the SFZ/3HNA co-crystal and the single component co-formers.

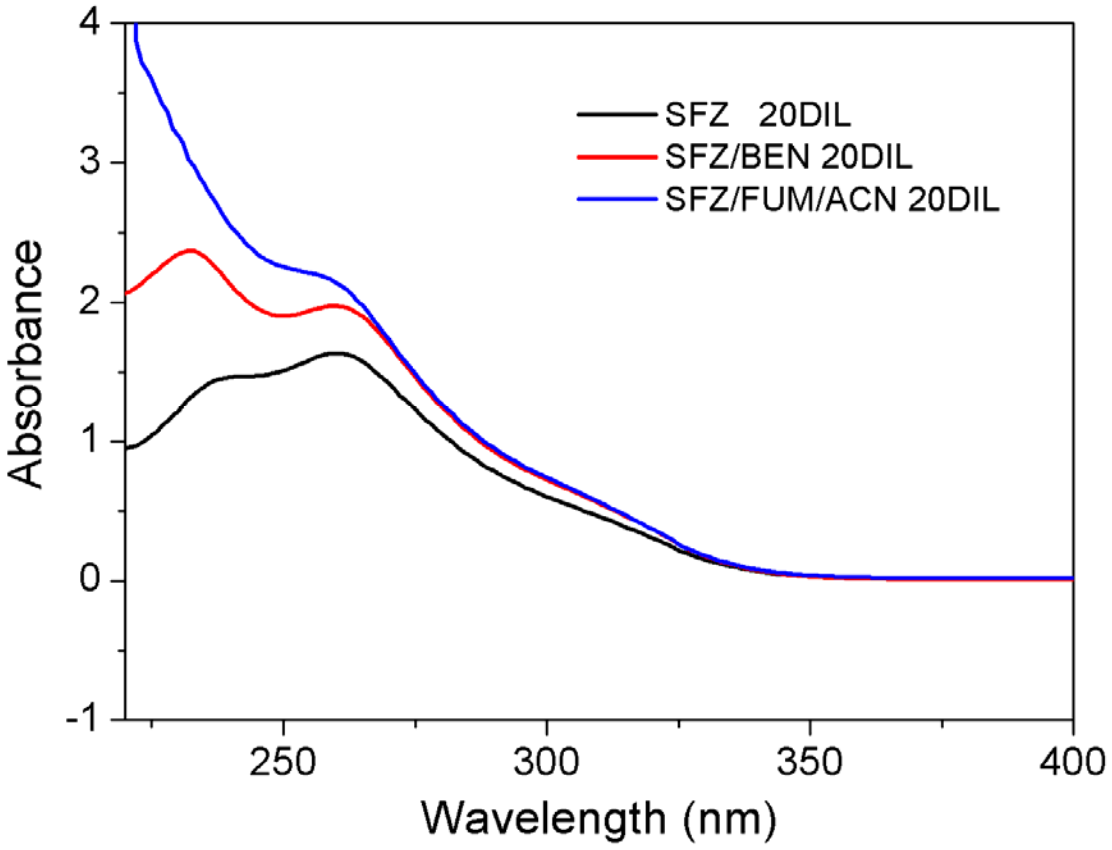

Figure S22. The UV absorption spectra of single component SFZ and SFZ/BEN and SFZ/FUM/ACN crystalline powder samples. The spectra were measured from 20 times diluted samples of the saturated solution obtained after 72 h stirring.