Supporting information

Spherical Cocrystallization - an enabling technology for the development of high dose direct compression tablets of poorly soluble drugs

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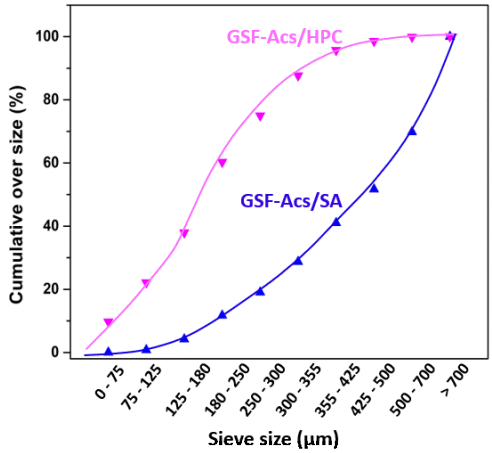

Figure S1. Particle size distribution of GSF-Acs/SA and GSF-Acs/HPC powders.

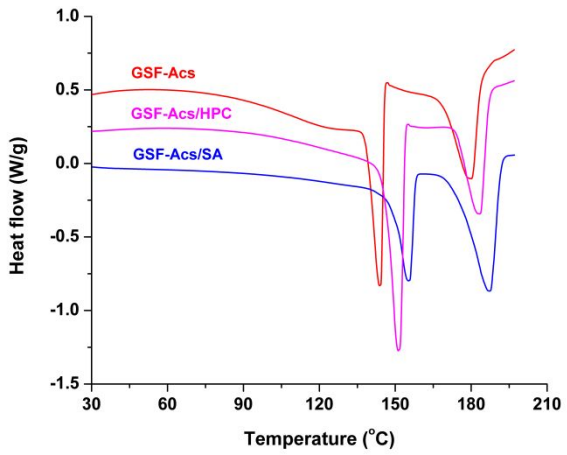

Figure S2. Thermal behavior of GSF-Acs, GSF-Acs/SA, and GSF-Acs/HPC characterized by differential scanning calorimetry.

Table S1. Intermolecular interaction energies estimated using B3LYP+D2/6+31G(d,p) dispersion corrected DFT model. Both the total energy ($E_{(tot)}$) and electrostatic ($E_{(ele)}$), polarization ($E_{(pol)}$), dispersion ($E_{(dis)}$), and exchange repulsion ($E_{(rep)}$) components of the energy are listed. R indicated the distance between centers of mass of the pair of molecules.

Sym. Op.	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
GSF (form I)						
x, y, z	8.90	-3.1	-1.6	-19.8	8.2	-16.7
-y, x, z+1/4	6.75	-9.2	-2.3	-32.1	23.6	-24.8
x, y, z	8.90	-2.2	-2.3	-11.0	11.6	-6.5
-y, x, z+1/4	7.00	-30.3	-12.0	-59.1	47.8	-62.9
y, -x, z+3/4	9.59	1.8	-2.7	-20.3	11.8	-10.6
-y, x, z+1/4	9.77	-11.6	-7.0	-23.7	18.0	-27.0
-x, -y, z+1/2	10.47	-11.2	-4.4	-19.3	13.6	-23.5
GSF-Acs cocrystal						
-	7.76	-38.7	-9.6	-5.6	47.1	-23.8
-	6.00	2.2	-1.1	-4.1	2.1	-0.7
-	6.71	0.1	-0.2	-0.8	0.0	-0.7
-	7.50	-41.0	-9.8	-6.9	46.2	-28.1
-	7.36	2.4	-0.7	-3.0	1.3	0.3
-	7.35	4.2	-0.5	-2.1	0.2	2.4
-	4.37	-10.6	-2.2	-4.9	4.1	-14.6
-	4.45	-96.9	-24.3	-7.6	107.9	-60.5
-	7.97	-8.3	-3.4	-9.3	2.8	-17.6
-	6.07	-17.8	-4.0	-39.2	26.1	-39.8
-	10.37	0.2	-0.4	-1.5	0.0	-1.5
x, y, z	8.71	4.4	-0.7	-2.3	0.4	2.4
-	4.45	-96.9	-24.3	-7.6	107.9	-60.5
-	7.66	-9.3	-5.4	-18.1	15.1	-20.2
-	7.25	-2.1	-1.6	-4.7	1.1	-6.7
-	7.61	-19.6	-4.8	-20.7	19.4	-30.3

-	5.55	-25.7	-8.7	-58.2	47.3	-55.0
-	4.37	-10.6	-2.2	-4.9	4.1	-14.6
x, y, z	13.62	-8.5	-2.9	-4.6	5.6	-11.7
x, y, z	8.71	-1.1	-3.7	-14.6	13.6	-8.2
-	8.29	2.9	-1.6	-17.5	7.5	-8.7
-	7.72	-20.1	-5.9	-34.7	26.9	-39.2
-	8.14	-16.2	-3.9	-26.5	13.2	-35.0
x, y, z	11.53	-12.2	-4.6	-10.9	11.3	-18.8
-x, y+1/2, -z	11.13	-0.1	-0.5	-5.4	2.0	-4.0
-	8.85	-16.1	-4.0	-29.3	16.8	-35.1
-	7.84	-20.6	-5.3	-54.7	43.7	-46.3
-	7.25	-2.1	-1.6	-4.7	1.1	-6.7
-	7.66	-9.3	-5.4	-18.1	15.1	-20.2
-	7.50	-41.0	-9.8	-6.9	46.2	-28.1
-	6.84	-1.2	-1.1	-25.7	13.8	-16.0
-	5.55	-25.7	-8.7	-58.2	47.3	-55.0
-	10.37	0.2	-0.4	-1.5	0.0	-1.5
-	7.36	2.4	-0.7	-3.0	1.3	0.3
-	7.35	4.2	-0.5	-2.1	0.2	2.4
x, y, z	8.71	0.6	-3.8	-14.5	15.2	-5.3
x, y, z	11.53	-16.4	-6.6	-18.4	17.9	-27.2
-x, y+1/2, -z	11.52	-0.1	-0.4	-3.8	0.5	-3.3
-	7.61	-19.6	-4.8	-20.7	19.4	-30.3
-	6.07	-17.8	-4.0	-39.2	26.1	-39.8
-	6.00	2.2	-1.1	-4.1	2.1	-0.7
-	7.97	-8.3	-3.4	-9.3	2.8	-17.6
-	7.76	-38.7	-9.6	-5.6	47.1	-23.8
-	6.71	0.1	-0.2	-0.8	0.0	-0.7