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Molecular simulation studies on the design of multicomponents Sorbic acid crystals for tuning solubility

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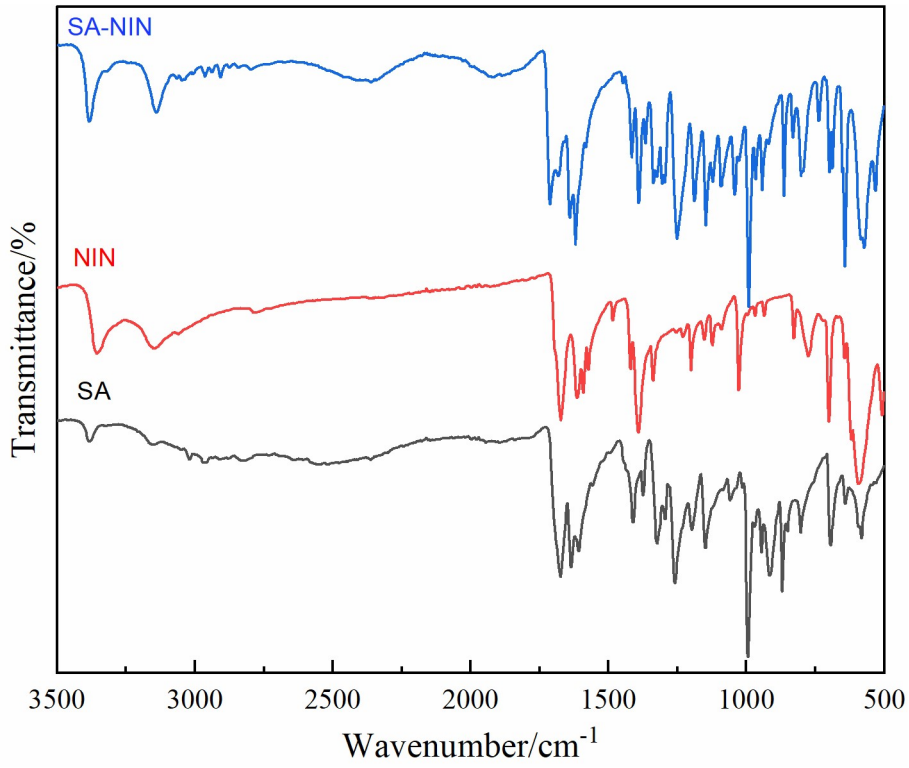

Figure S1. FTIR spectra of SA, NIA and SA-NIA.

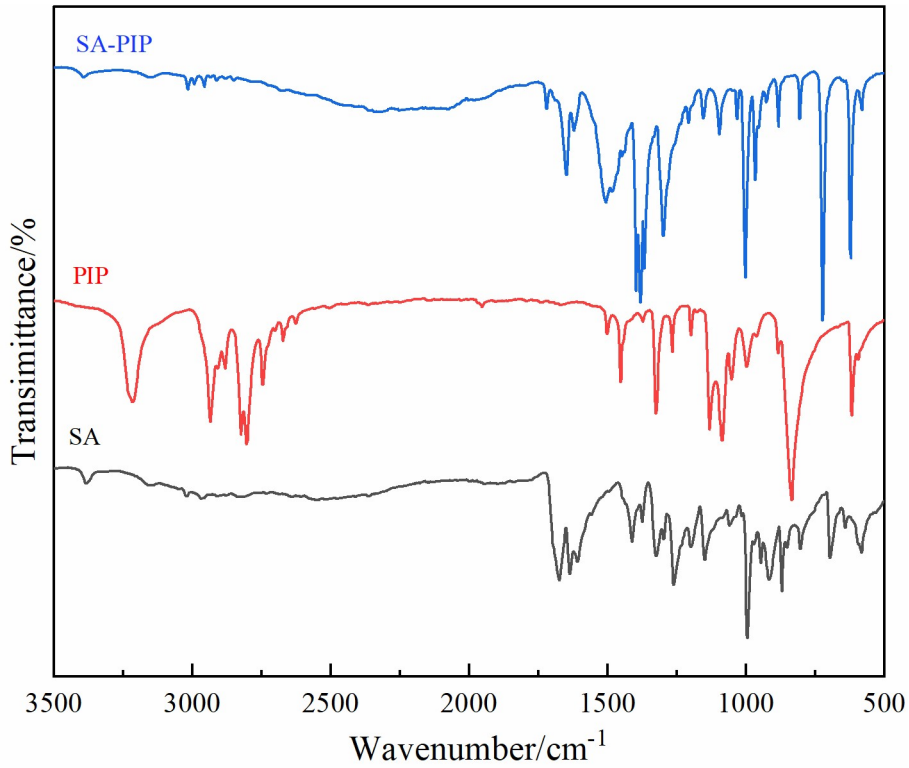

Figure S2. FTIR spectra of SA, PIP and SA-PIP.

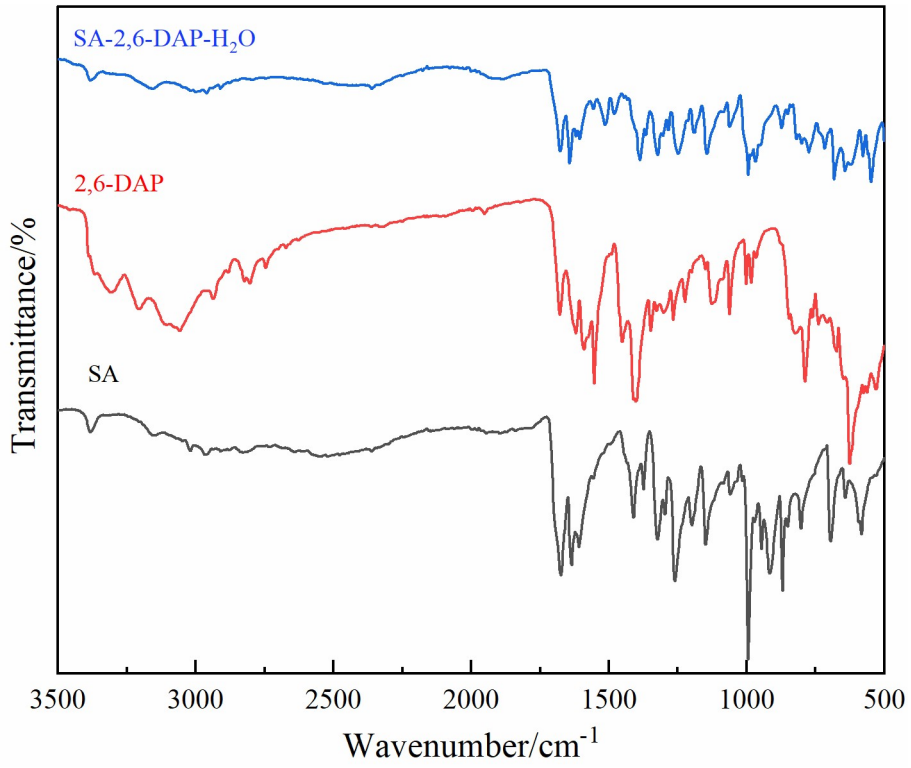

Figure S3. FTIR spectra of SA, 2,6-DAP and SA-2,6-DAP-H_2O.

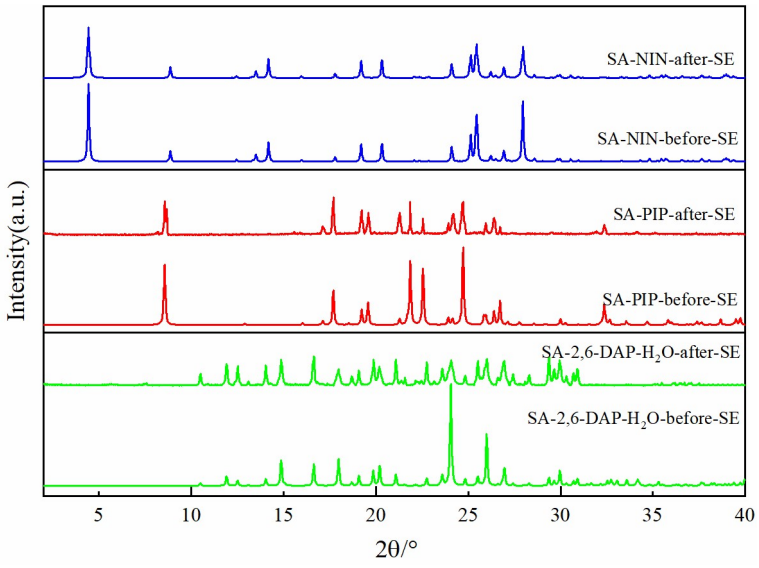

Figure S4. PXRD patterns of SA and its multicomponent crystals before and after equilibrium solubility experiments (SE).

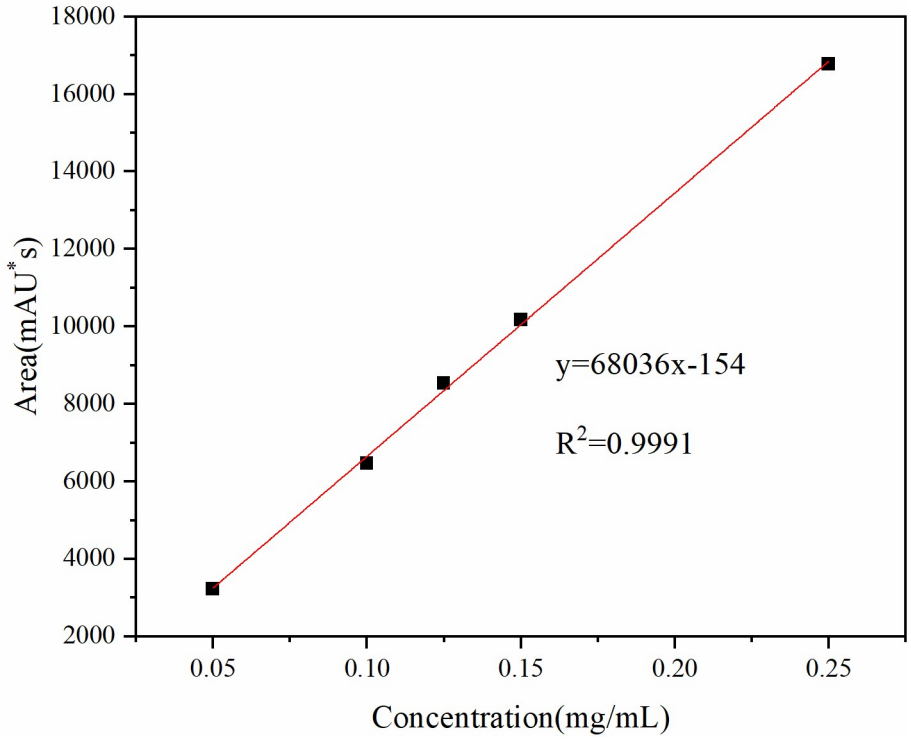

Figure S5. HPLC standard curve of SA.

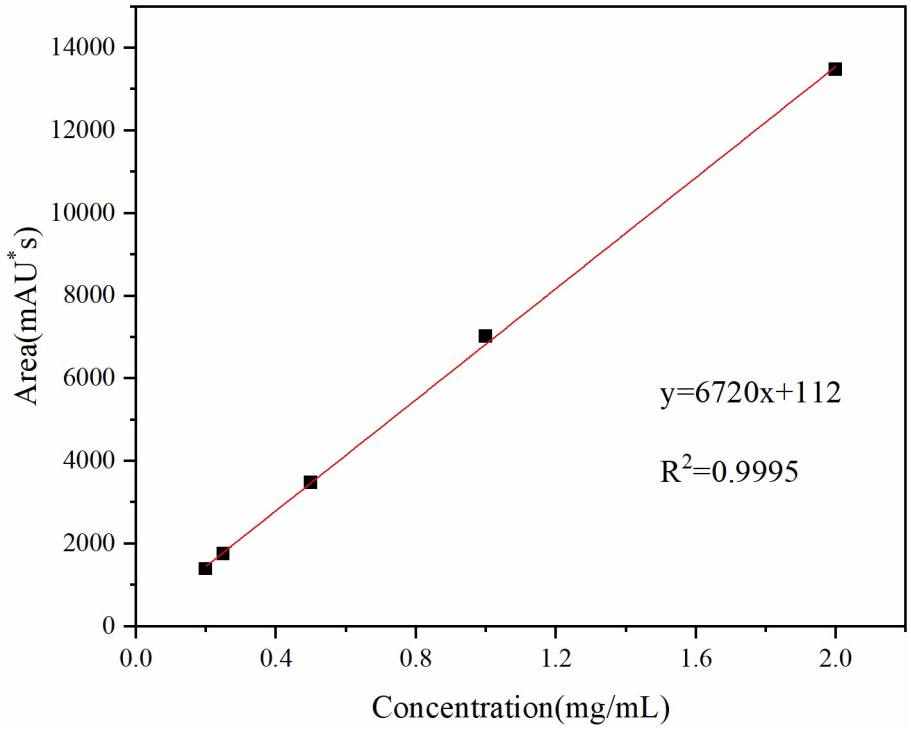

Figure S6. HPLC standard curve of NIA.

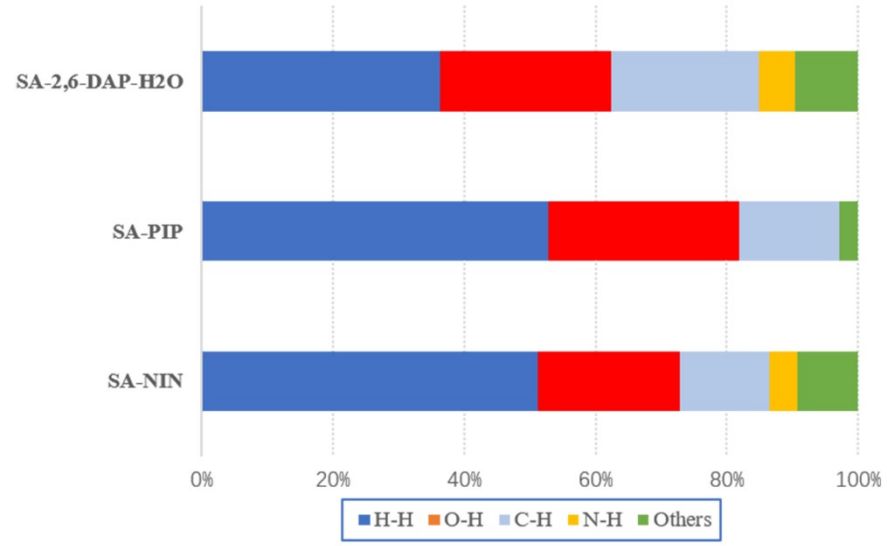

Figure S7. Percentage contributions of molecular contact interactions to the Hirshfield surface in three multicomponent crystals.

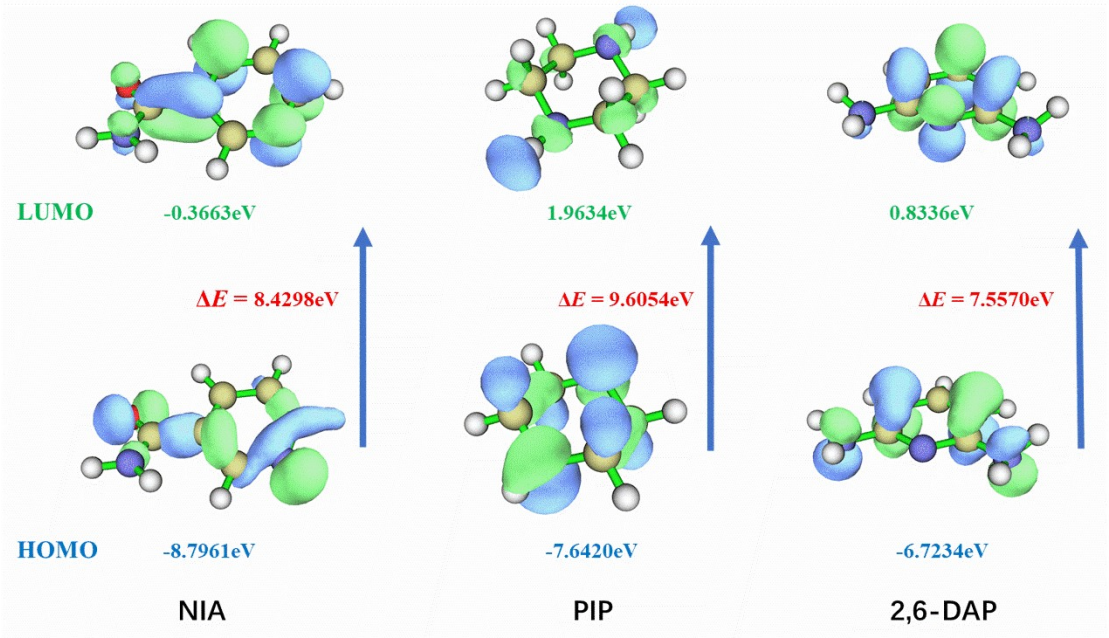

Figure S8. HOMO–LUMO plot of NIA, PIP and 2,6-DAP with orbital involved in electronic transitions.

Table S1. SA, Salt/Cocrystal FTIR Stretching Frequency

compound	-C=O(cm^{-1})	-OH (cm^{-1})	-NH (cm^{-1})
SA	1674	3383	/
NIA	1674	/	3354
PIP	/	/	3216
2,6-DAP	/	/	3206
SA- NIA	1641	3383	3140
SA- PIP	1647	3391	3016

SA-2,6-DAP-H_2O	1643	3381	3156

Table S2. Parameters (Å, Degree) of the Hydrogen Bonds for Multicomponent Crystals of SA.

D−H···A	D−H	H··· A	D··· A	D−H···A	symmetry
SA-NIA					
O_2−H_2···N_1	1.01	1.62	2.63	175	
N_2−H_{2C}···O_1	0.90	2.15	3.04	172	-1+x, y, z
N_2−H_{2B}···O_3	0.91	1.97	2.88	176	-1-x,1-y,1-z
C_{11}−H_{11}···O_1	0.95	2.57	3.40	146	x, -1+y, z
SA-PIP					
N_1−H_{1A}···O_1	0.97	1.71	2.68	177	
N_1−H_{1A}···O_2	0.97	2.52	3.16	123	
N_1−H_{1B}···O_2	0.99	1.69	2.67	173	-1+x, y, z
C_2−H_2···O_1	0.93	2.56	3.49	174	1+x, y, z
C_3−H_3···O_1	0.93	2.50	2.82	100	
C_7−H_{7A}···O_1	0.97	2.37	3.33	169	-x,1-y,1-z
SA-2,6-DAP-H_2O					
N_1−H_1···O_2	0.92	1.82	2.74	178	
N_2−H_{2A}···O_3	0.90	1.99	2.89	172	-1/2+x,1/2-y,1/2+z
N_2−H_{2B}···O_1	0.91	1.99	2.90	178	
N_3−H_{3A}···O_3	0.90	2.07	2.96	171	
N_3−H_{3B}···O_1	0.89	2.19	3.04	159	-1/2+x,1/2-y, -1/2+z
O_3−H_{3C}···O_2	0.89	1.84	2.68	158	
O_3−H_{3D}···O_1	0.86	1.89	2.73	169	3/2-x, -1/2+y,3/2-z

Table S3. Experimental solid–liquid equilibrium data (mass fraction) for SA-NIA at 20℃and 30℃and pressure p = 101.3 kPa.[a]

	Mass fraction			
T/℃	SA	NIA	EtOH	Equilibrium solid phase [b]
20	0	0.10944	0.89056	NIA
	0.02242	0.11059	0.86699	NIA
	0.05273	0.10938	0.83789	NIA
	0.06245	0.10684	0.83071	NIA+1:1SA-NIA
	0.06972	0.09998	0.8303	1:1SA-NIA
	0.09215	0.06287	0.84499	1:1SA-NIA
	0.10266	0.05759	0.83976	1:1SA-NIA
	0.11828	0.04771	0.83401	SA+1:1SA-NIA
	0.12356	0.04049	0.83595	SA
	0.12684	0	0.87316	SA
30	0	0.11823	0.88177	NIA
	0.02158	0.12365	0.85477	NIA
	0.0631	0.12694	0.80996	NIA
	0.07318	0.12189	0.80493	NIA+1:1SA-NIA
	0.08000	0.11214	0.80786	1:1SA-NIA
	0.11137	0.07722	0.81141	1:1SA-NIA
	0.13871	0.06069	0.8006	SA+1:1SA-NIA
	0.14337	0.04538	0.81125	SA
	0.12986	0	0.87014	SA

[a] Standard uncertainty u is u(T) = 0.01 K, u(p) = 10 kPa; the relative standard uncertainty of mass fraction u_r(x) = 0.05.

[b] Mole ratio of SA-to-NIA in cocrystal is 1:1.