

Supplementary Information

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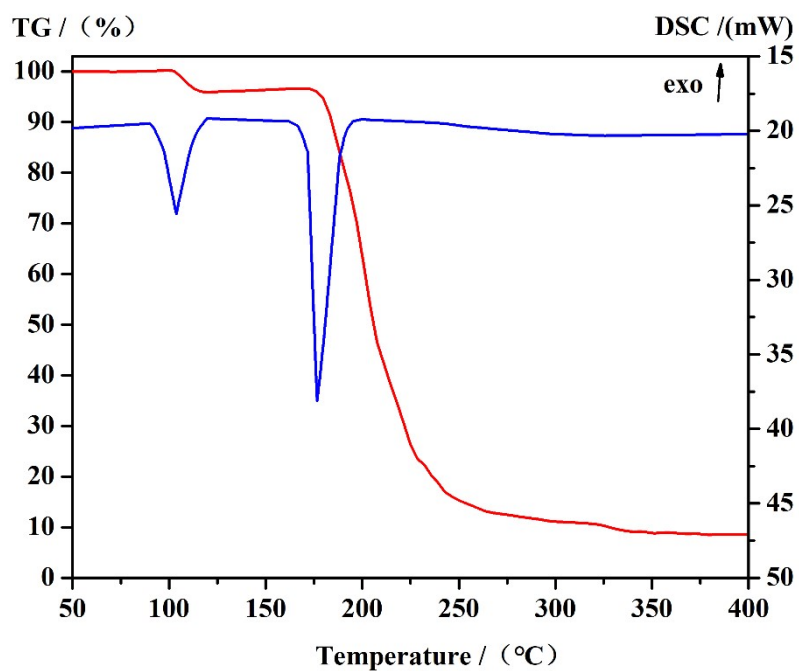


Figure S1 DSC (blue line) and TG (red line) profiles of PCI-FA.

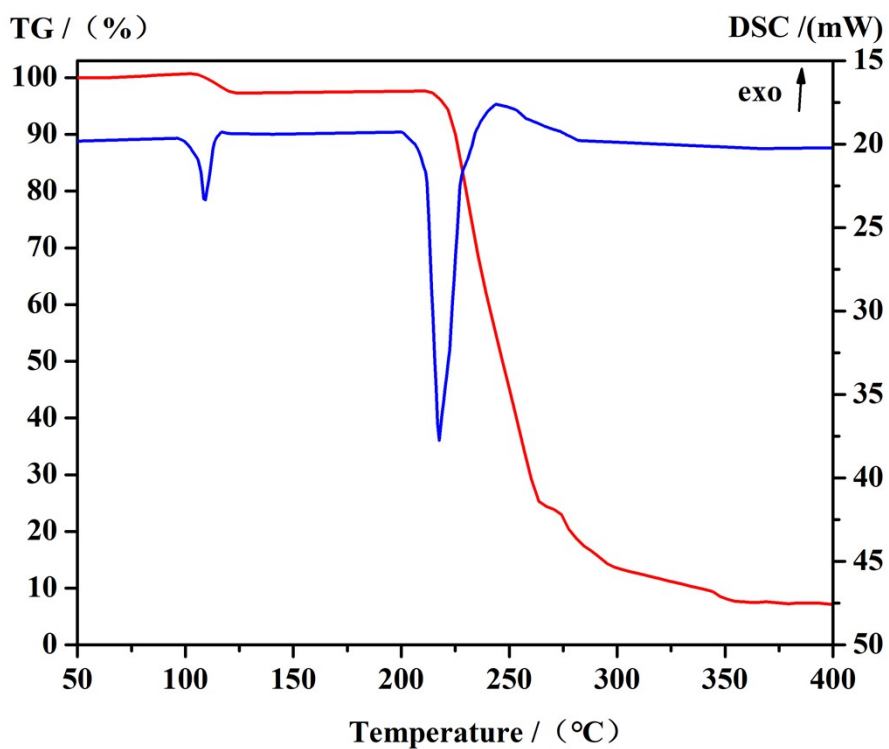


Figure S2 DSC (blue line) and TG (red line) profiles of PCI-VA.

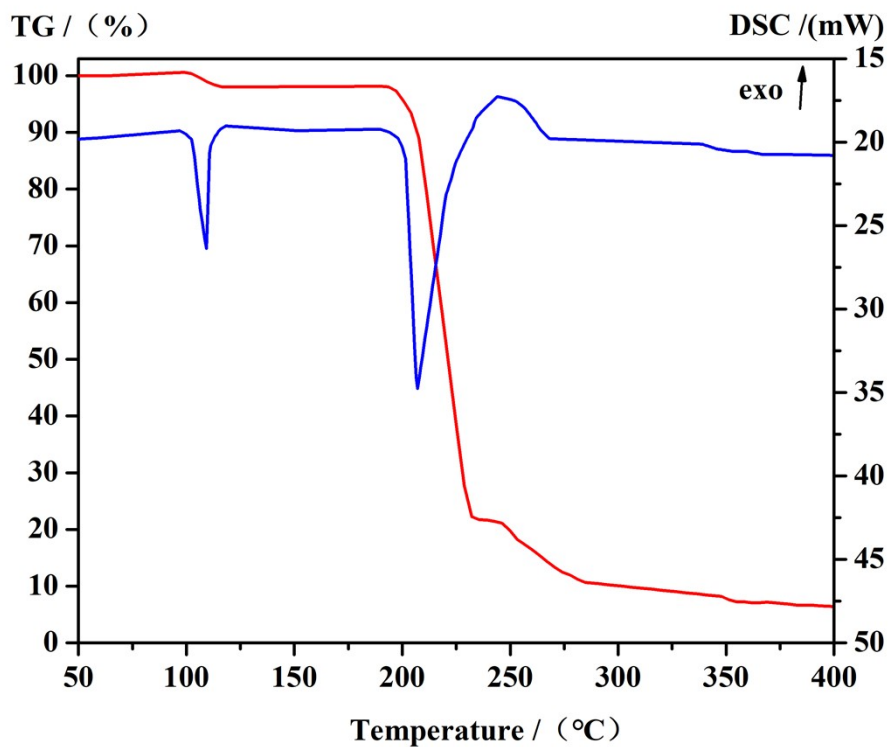


Figure S3 DSC (blue line) and TG (red line) profiles of PCI-SA.

Sample	RH Condition	Replicate	Initial Mass (mg)	Final Mass (mg)	Moisture Uptake (%)	Average Hygroscopicity (%)
PCI	75% RH	1	50.02	53.59	7.13	-
		2	50.15	53.72	7.12	-
		3	49.98	53.58	7.14	7.13
	80% RH	1	50.01	58.97	17.92	-
		2	50.1	58.98	17.92	-
		3	49.95	58.96	17.93	17.92
	98% RH	1	50.02	59.94	19.92	-
		2	50.15	59.95	19.92	-
		3	49.98	59.93	19.94	19.93
PCI-FA	75% RH	1	50.05	51.4	2.81	-
		2	50.1	51.41	2.81	-
		3	49.95	51.39	2.82	2.81
	80% RH	1	50.03	51.81	3.61	-
		2	50.08	51.82	3.61	-
		3	49.95	51.8	3.62	3.61
	98% RH	1	50.05	52.07	4.15	-
		2	50.1	52.08	4.15	-

Table S1. Average Hygroscopicity of PCI, PCI-FA, PCI-SA, and PCI-VA at Different RH Conditions.

Sample	RH Condition	Replicate	Initial Mass (mg)	Final Mass (mg)	Moisture Uptake (%)	Average Hygroscopicity (%)
PCI-SA	75% RH	3	49.95	52.06	4.16	4.15
		1	50.08	51.89	3.79	-
		2	50.12	51.9	3.79	-
	80% RH	3	49.92	51.88	3.8	3.79
		1	50.05	52.19	4.38	-
		2	50.1	52.2	4.38	-
	98% RH	3	49.92	52.18	4.39	4.38
		1	50.08	52.64	5.25	-
		2	50.12	52.65	5.25	-
PCI-VA	75% RH	3	49.92	52.63	5.26	5.25
		1	50	52.19	4.39	-
		2	50.05	52.2	4.39	-
	80% RH	3	49.9	52.18	4.4	4.39
		1	50	52.7	5.41	-
		2	50.05	52.71	5.41	-
	98% RH	3	49.9	52.69	5.42	5.41
		1	50	53.28	6.57	-
		2	50.05	53.29	6.57	-
		3	49.9	53.27	6.58	6.57

Continued Table S1. Average Hygroscopicity of PCI, PCI-FA, PCI-SA, and PCI-VA at Different RH Conditions.



Fig. S4 Solvent Negative Controls for *E. coli*, *S. aureus* and *B. subtilis*.

Table S2. Antibacterial Activity of PCI-FA, PCI-VA, PCI-SA Cocrystals and their Physical Mixtures against *E.coli*.

Bacterial strain	Diameter of inhibition zone (mm)			
	<i>E.coli</i>			
Drug concentration (mg/mL)	5	2.5	1.25	0.63
Number on desk	1	2	3	4
PM1	16.1±0.1	13.0±0.1	9.3±0.2	8.0±0.2
PM2	16.0±0.1	15.7±0.1	9.0±0.1	8.0±0.2
PM3	15.0±0.1	12.9±0.1	8.3±0.2	7.5±0.2
PCI-FA	24.5±0.1	22.3±0.2	20.0±0.1	18.3±0.2
PCI-VA	22.9±0.2	22.0±0.1	19.0±0.1	17.0±0.1
PCI-SA	21.1±0.2	20.0±0.1	17.5±0.1	15.1±0.2

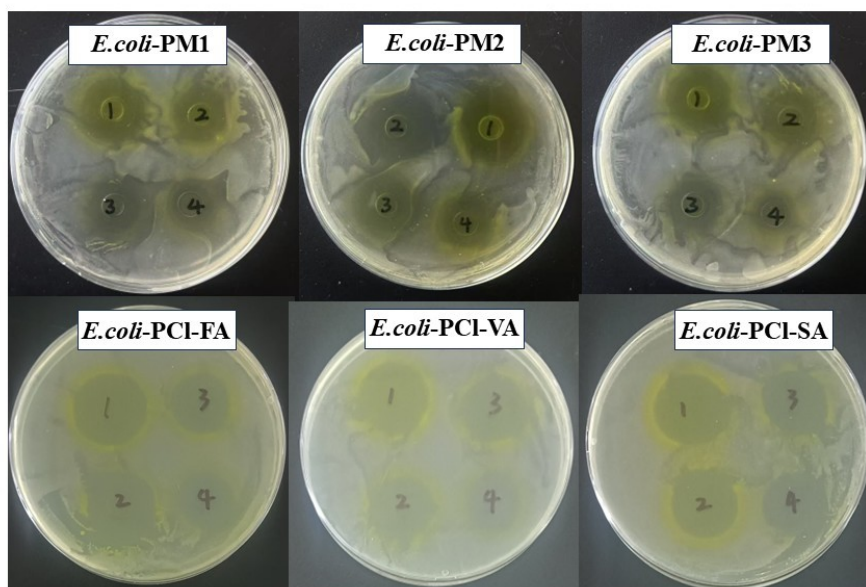


Fig. S5 Oxford Cup Test Results of PCI-FA, PCI-VA, PCI-SA Cocrystals and their Physical Mixtures on *E. coli*.

Table S3. Antibacterial Activity of PCI-FA, PCI-VA, PCI-SA Cocrystals and their Physical

Mixtures against *S.aureus*.

		Diameter of inhibition zone (mm)			
Bacterial strain	<i>S.aureus</i>				
Drug concentration (mg/mL)	5	2.5	1.25	0.63	
Number on desk	1	2	3	4	
PM1	16.0±0.1	15.6±0.1	14.0±0.2	9.0±0.2	
PM2	16.0±0.1	15.7±0.1	14.2±0.1	8.7±0.1	
PM3	15.0±0.1	14.3±0.2	14.0±0.1	8.3±0.1	
PCI-FA	22.7±0.2	22.0±0.1	17.7±0.2	12.7±0.1	
PCI-VA	20.7±0.1	20.2±0.1	18.2±0.2	12.0±0.2	
PCI-SA	20.0±0.2	19.7±0.1	15.3±0.1	11.7±0.2	

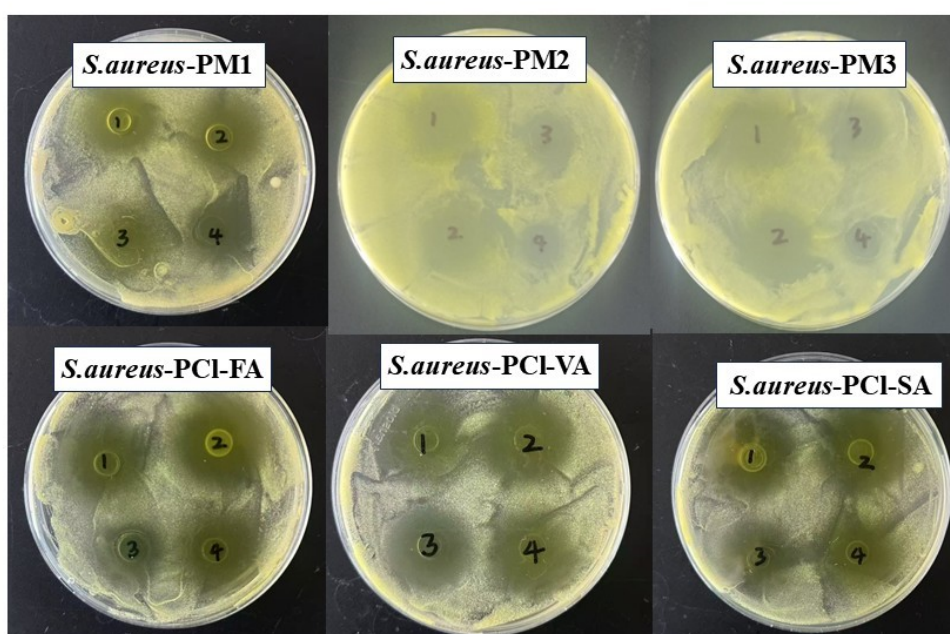


Fig. S6 Oxford Cup Test Results of PCI-FA, PCI-VA, PCI-SA Cocrystals and their Physical Mixtures on *S.aureus*.

Table S4. Antibacterial Activity of PCI-FA, PCI-VA, PCI-SA Cocrystals and their Physical Mixtures against *B.subtilis*.

Bacterial strain	Diameter of inhibition zone (mm)			
	<i>B.subtilis</i>			
Drug concentration (mg/mL)	5	2.5	1.25	0.63
Number on desk	1	2	3	4
PM1	16.0±0.1	13.0±0.1	12.0±0.2	9.3±0.2
PM2	15.8±0.2	12.7±0.2	11.0±0.1	9.0±0.1
PM3	11.5±0.1	10.6±0.1	10.1±0.1	7.9±0.2
PCI-FA	24.5±0.2	23.7±0.1	21.0±0.1	17.8±0.1
PCI-VA	22.0±0.1	20.0±0.1	19.0±0.2	17.0±0.2
PCI-SA	20.0±0.2	16.1±0.1	15.5±0.1	15.0±0.1

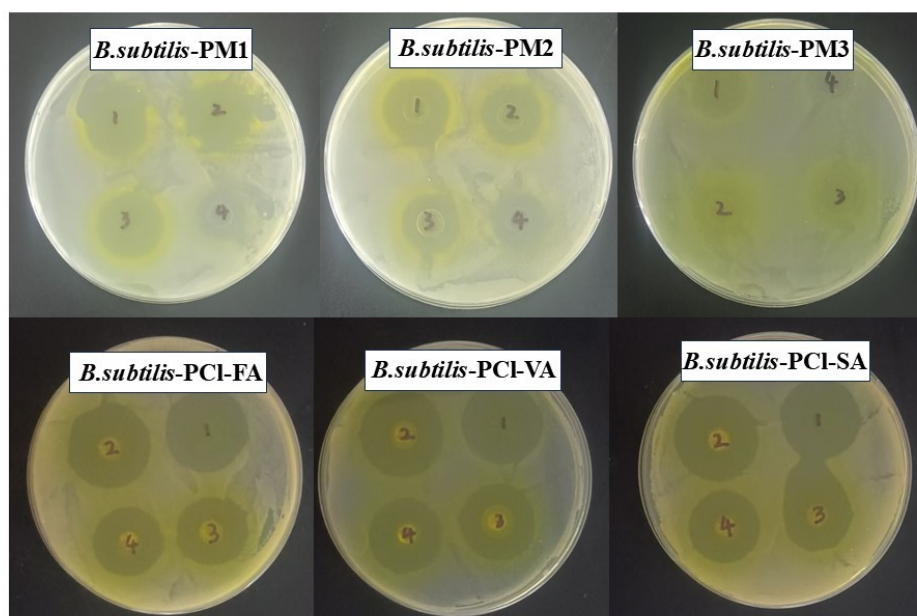


Fig. S7 Oxford Cup Test Results of PCI-FA, PCI-VA, PCI-SA Cocrystals and their Physical Mixtures on *B.subtilis*.