Supplementary Material (ESI) for CrystEngComm

Purification of Amoxicillin Trihydrate by Impurity-Coformer Complexation in Solution

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1. Complete List of Forty-Seven Compounds Used in Coformer Screening:

Table 1 Compounds with Amide, Primary, Secondary, and Tertiary Amine Group

(Group I)

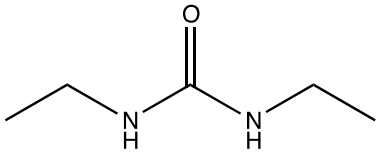
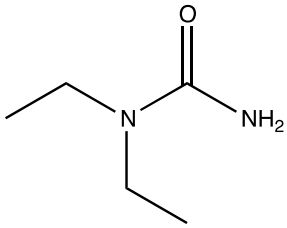
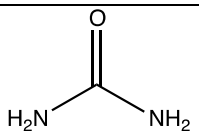
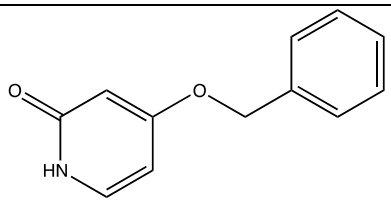
Name	Molecular Weight	Structure
1,3 diethylruea	116.16	
1,1 diethylurea	116.16	
Urea	60.56	
4-benzyloxy-2(1H)-pyridone	201.22	

Table 2 Compounds with Amide, Primary, Secondary, and Tertiary Amine Group

(Group I) (Cont'd)

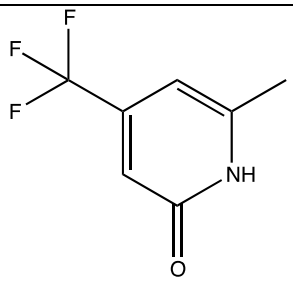
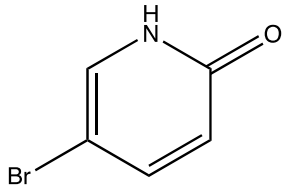
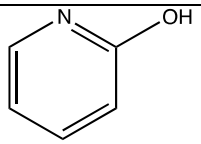
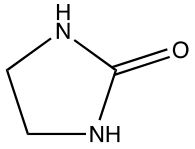
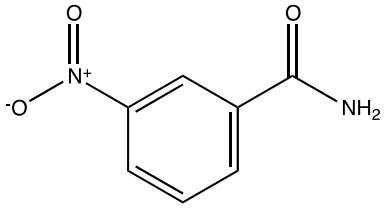
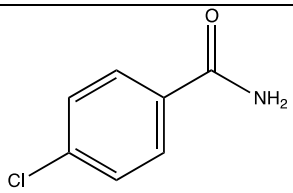
6-methyl-4-(trifluoromethyl)-2(1H)-pyridone	177.12	
5-bromo-2(1H)-pyridone	174	
2-hydroxypyridine	95.1	
2-imidazolidone	86.09	
3-nitrobenzamide	166.13	
4-chlorobenzamide	155.58	

Table 3 Compounds with Amide, Primary, Secondary, and Tertiary Amine Group

(Group I) (Cont'd)

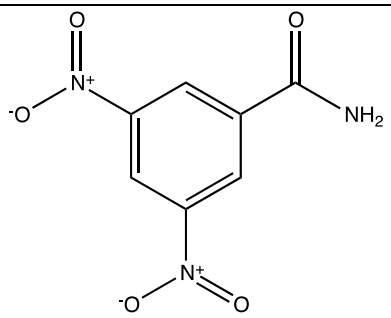
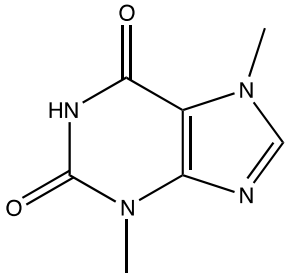
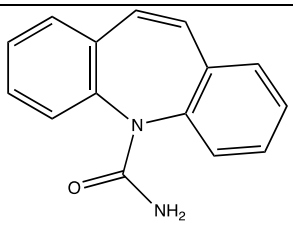
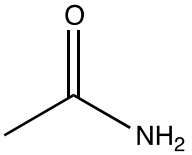
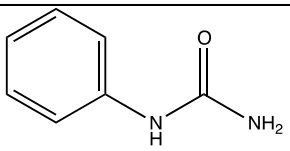
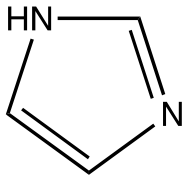
3,5-dinitrobenzamide	211.13	
Theobromine	180.16	
Carbamazepine	236.27	
Acetamide	59.07	
N-phenylurea	136.15	
Imidazole	68.08	

Table 4 Compounds with Amide, Primary, Secondary, and Tertiary Amine Group

(Group I) (Cont'd)

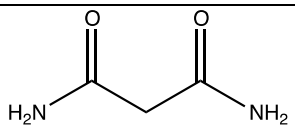
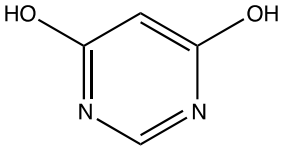
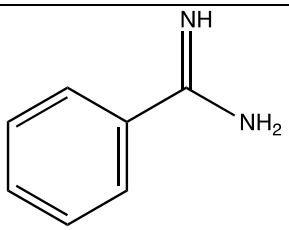
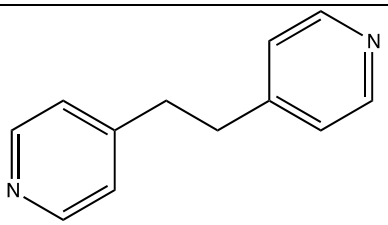
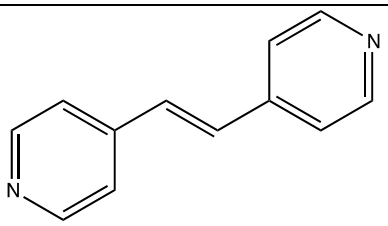
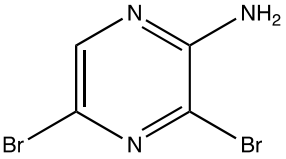
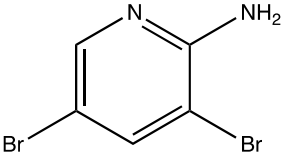
Malonamide	102.09	
4,6-dihydroxypyrimidine	112.09	
Benzamidine	120.15	
1,2-bis(4-pyridyl)ethane	184.24	
1,2-di(4-pyridyl)ethylene	182.22	
2-amino-3,5-dibromopyrazine	252.89	
2-amino-3,5-dibromopyridine	251.91	

Table 5 Compounds with Amide, Primary, Secondary, and Tertiary Amine Group

(Group I) (Cont'd)

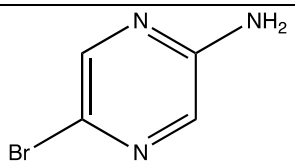
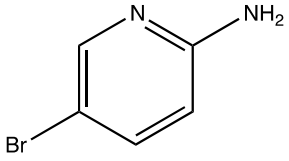
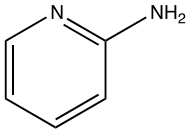
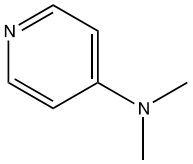
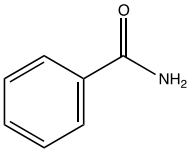
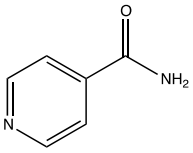
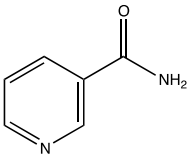
2-amino-5-bromopyrazine	174.00	
2-amino-5-bromopyridine	173.01	
2-aminopyridine	94.11	
4-(dimethylamino)-pyridine	122.17	
Benzamide	121.14	
Isonicotinamide	122.12	
Nicotinamide	122.12	

Table 6 Compounds with Amide, Primary, Secondary, and Tertiary Amine Group

(Group I)(Cont'd)

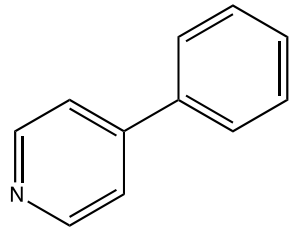
4-phenylpyridine	155.20	

Table 7 Compounds with Carboxylic Acid Group (Group II)

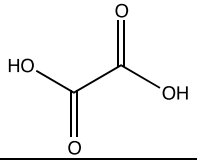
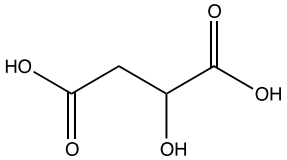
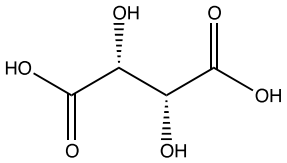
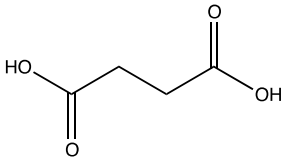
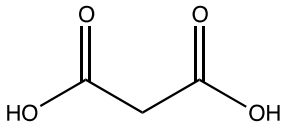
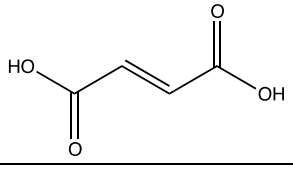
Name	Molecular Weight	Structure
Oxalic acid	90.03	
L-malic acid	134.09	
L-tartaric acid	150.087	
Succinic acid	118.09	
Malonic acid	104.06	
Fumaric acid	116.07	

Table 8 Compounds with both Carboxylic Acid and Amine Group (Group III)

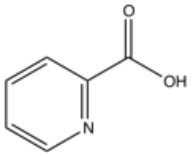
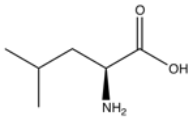
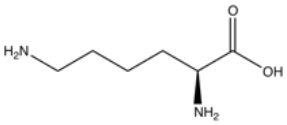
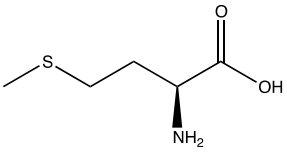
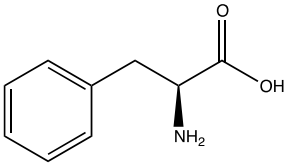
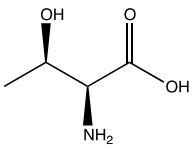
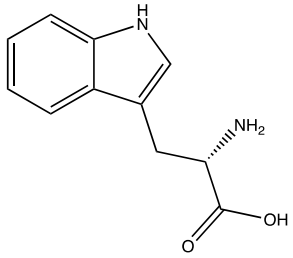
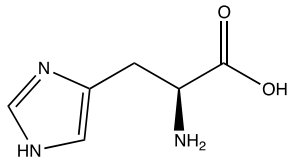
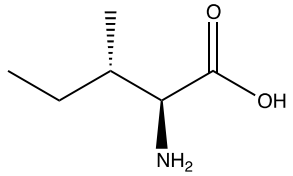
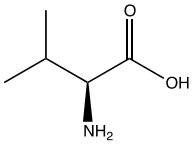
Name	Molecular Weight	Structure
2-picolinic acid	123.11	
L-leucine	131.17	
L-Lysine	146.19	
L-methionine	149.21	
L-phenylalanine	165.19	
L-threonine	119.12	

Table 9 Compounds with both Carboxylic Acid and Amine Group (Group III) (Cont'd)

L-tryptophan	204.23	
L-histidine	155.15	
L-isoleucine	131.17	
L-valine	117.15	

2. X-ray Powder Diffraction Patterns for 4HPG Cocrystals:

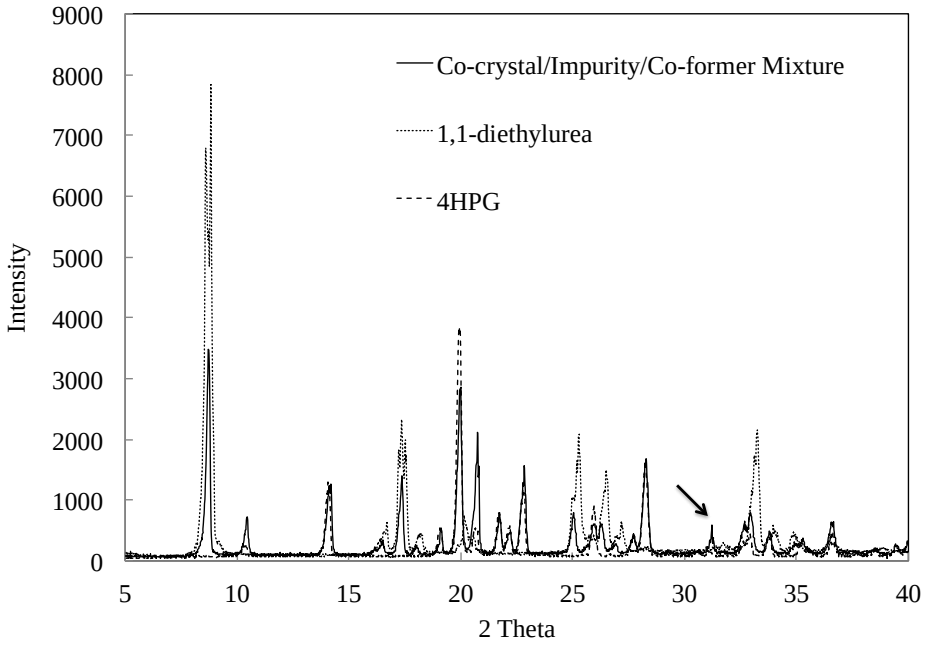


Figure 1 The Comparison between the Powder Pattern of the Cocrystal/4HPG/1,1-diehtylurea Mixture and the Powder Patterns of the Individual Components.

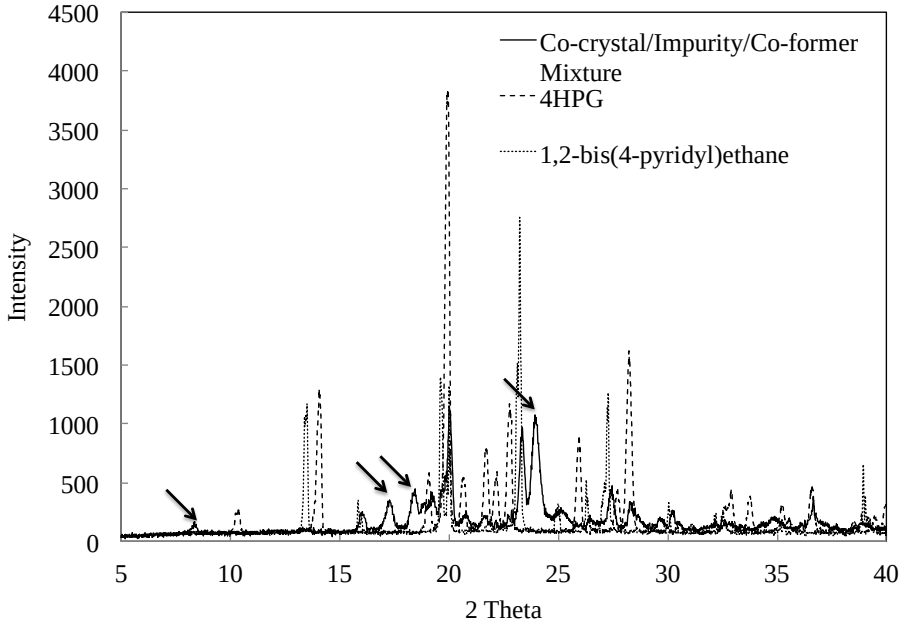


Figure 2 The Comparison between the Powder Pattern of the Cocrystal/4HPG/1,2-bis(4-pyridyl)ethane Mixture and the Powder Patterns of the Individual Components.

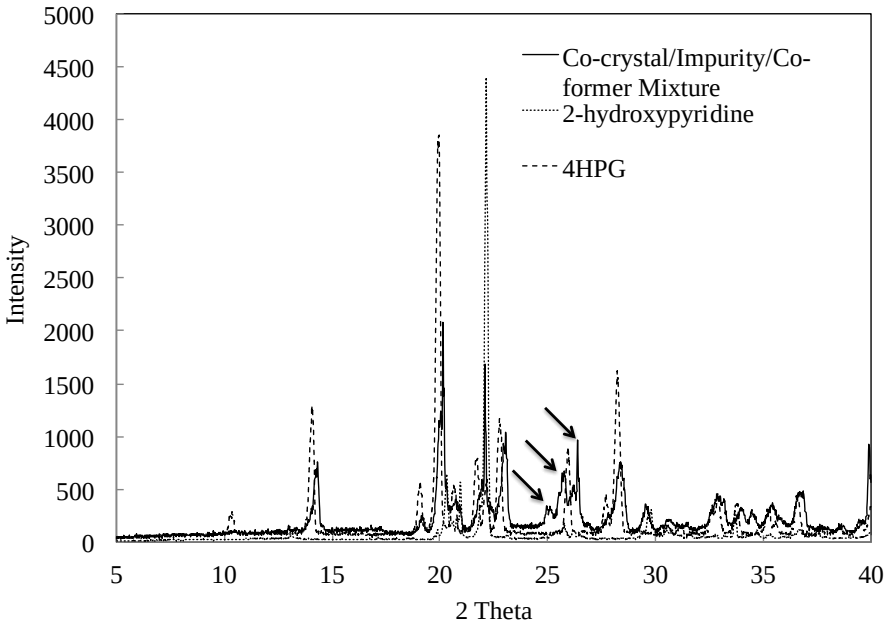


Figure 3 The Comparison between the Powder Pattern of the Cocrystal/4HPG/2-hydroxypyridine and the Powder Patterns of the Individual Components.

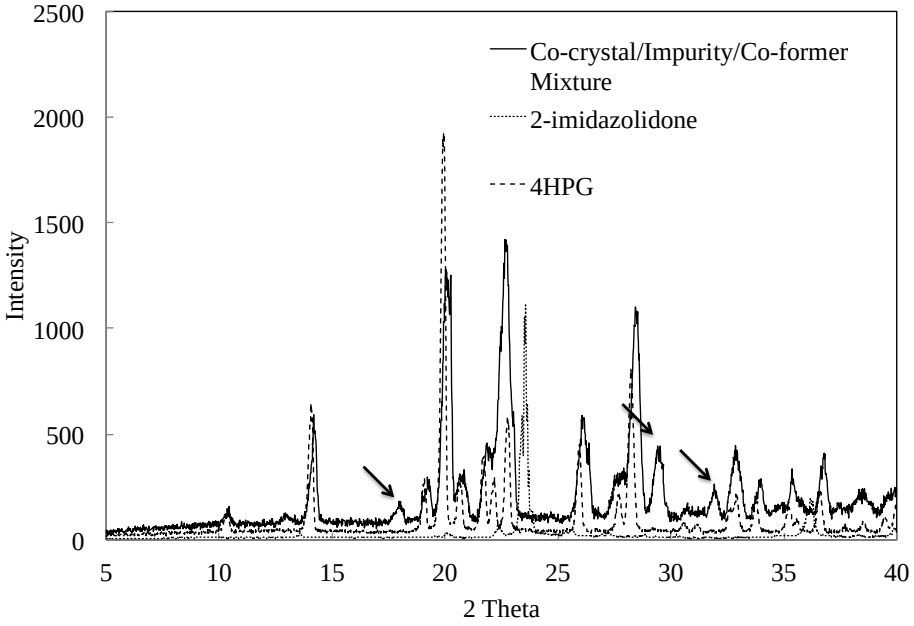


Figure 4 The Comparison between the Powder Pattern of the Cocrystal/4HPG/2-imidazolidone Mixture and the Powder Patterns of the Individual Components.

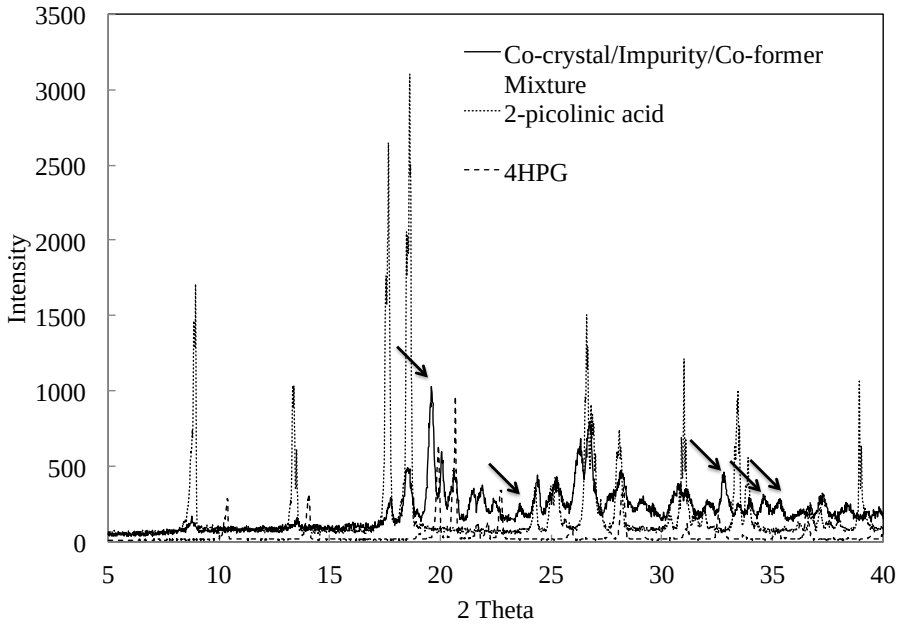


Figure 5 The Comparison between the Powder Pattern of the Cocrystal/4HPG/2-picolinic acid Mixture and the Powder Patterns of the Individual Components.

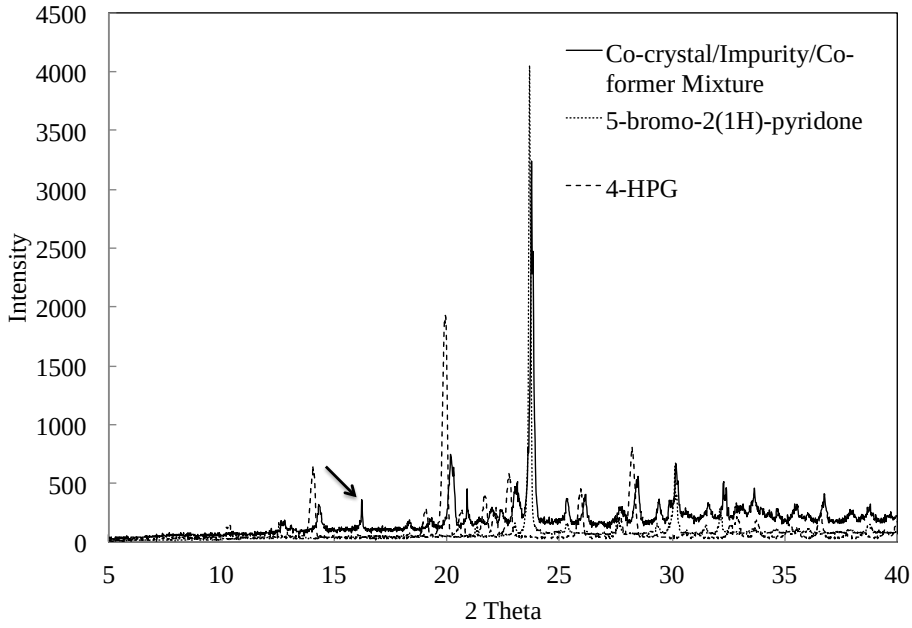


Figure 6 The Comparison between the Powder Pattern of the Cocrystal/4HPG/5-bromo-2(1H)-pyridone Mixture and the Powder Patterns of the Individual Components.

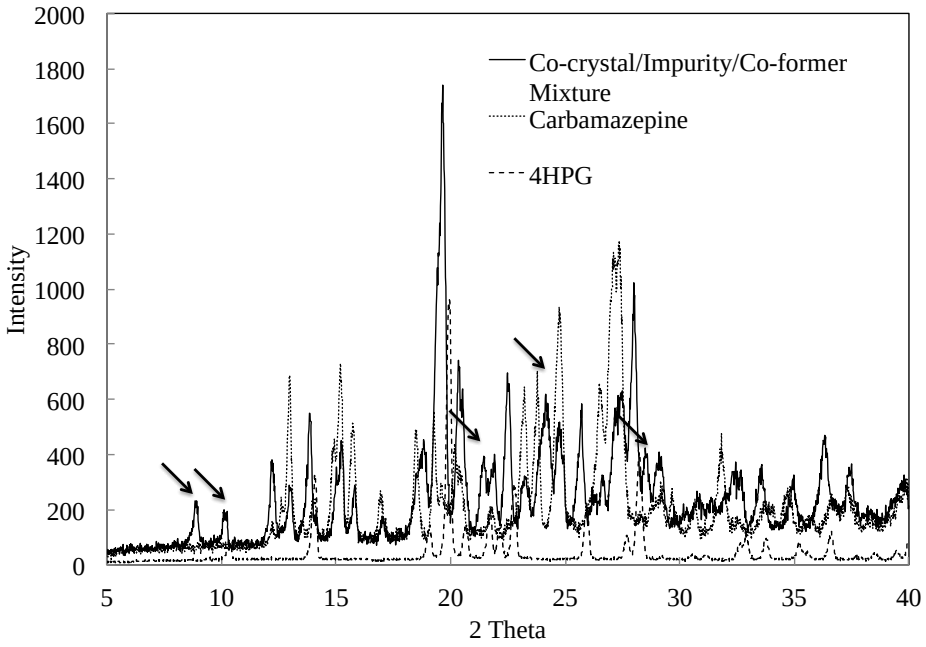


Figure 7 The Comparison between the Powder Pattern of the Cocrystal/4HPG/Carbamazepine Mixture and the Powder Patterns of the Individual Components.

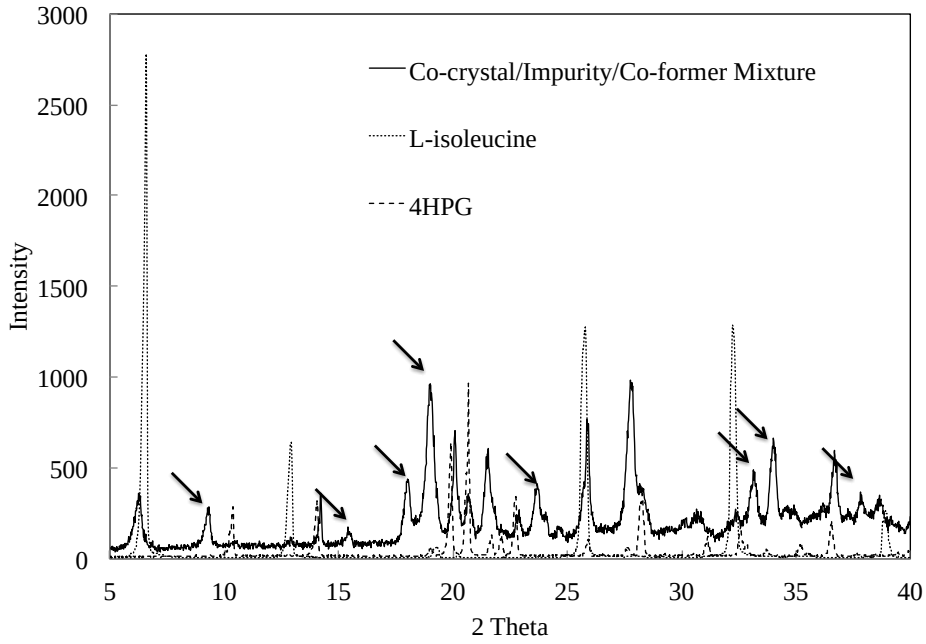


Figure 8 The Comparison between the Powder Pattern of the Cocrystal/4HPG/L-isoleucine Mixture and the Powder Patterns of the Individual Components.

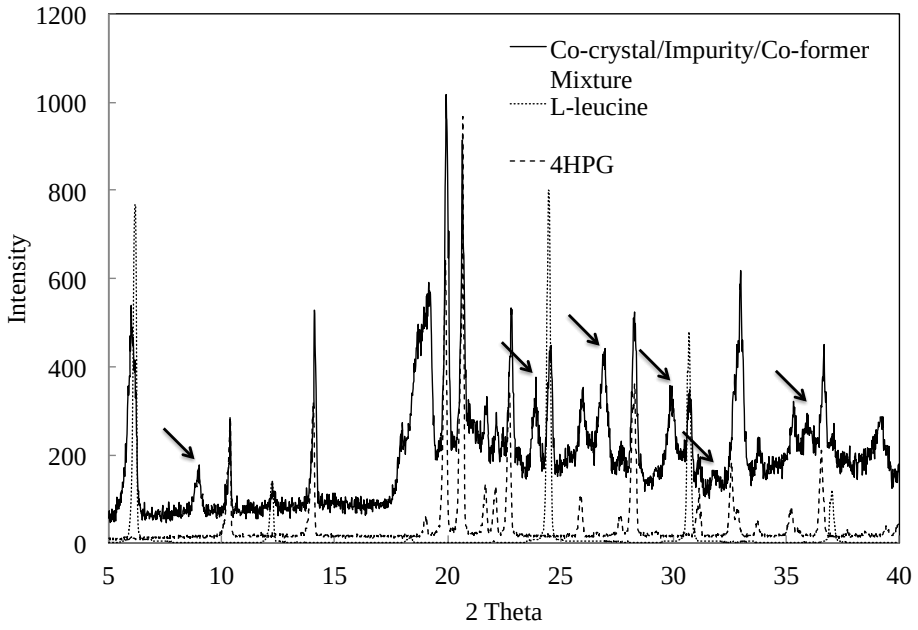


Figure 9 The Comparison between the Powder Pattern of the Cocrystal/4HPG/L-leucine Mixture and the Powder Patterns of the Individual Components.

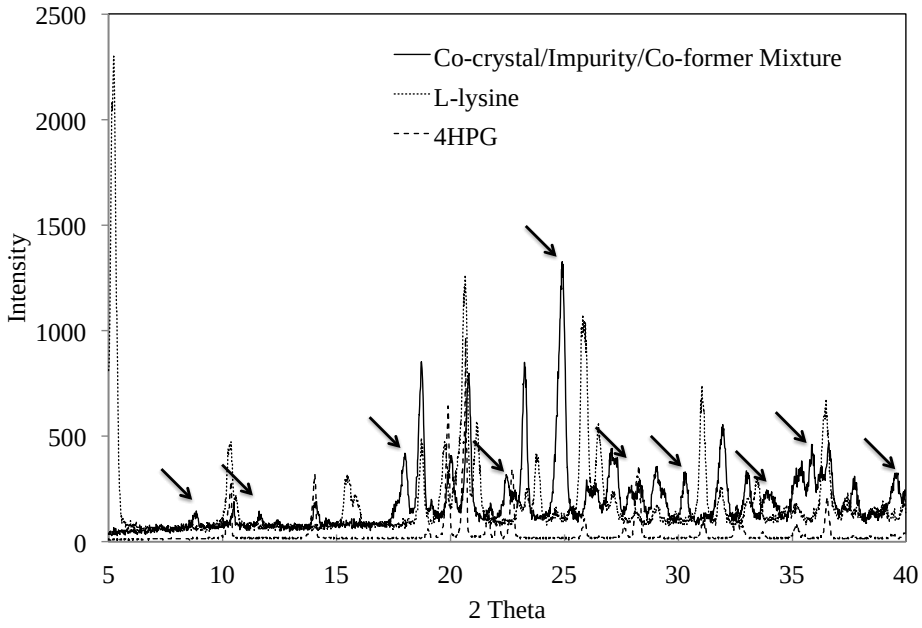


Figure 10 The Comparison between the Powder Pattern of the Cocrystal/4HPG/L-lysine Mixture and the Powder Patterns of the Individual Components.

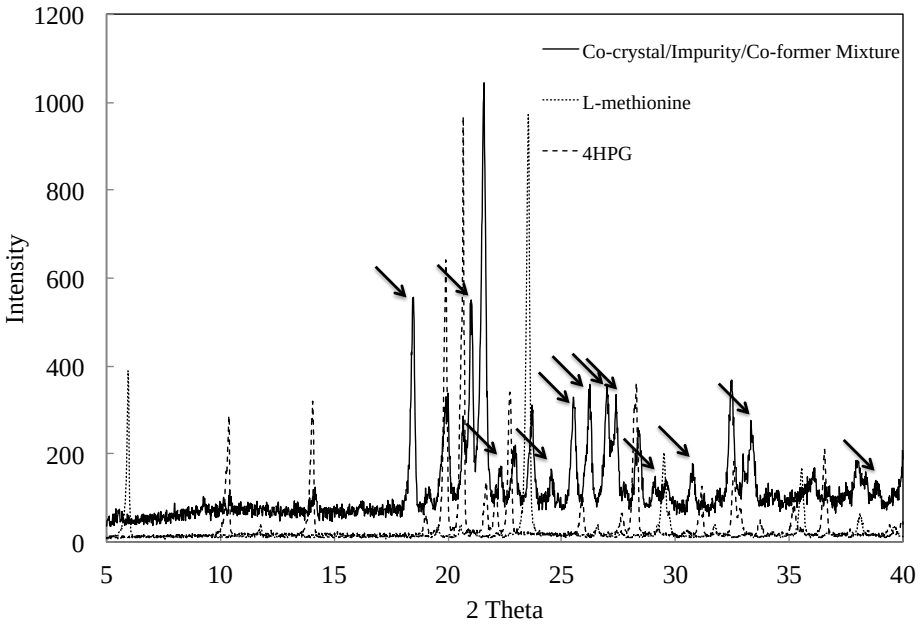


Figure 11 The Comparison between the Powder Pattern of the Cocrystal/4HPG/L-methionine Mixture and the Powder Patterns of the Individual Components.

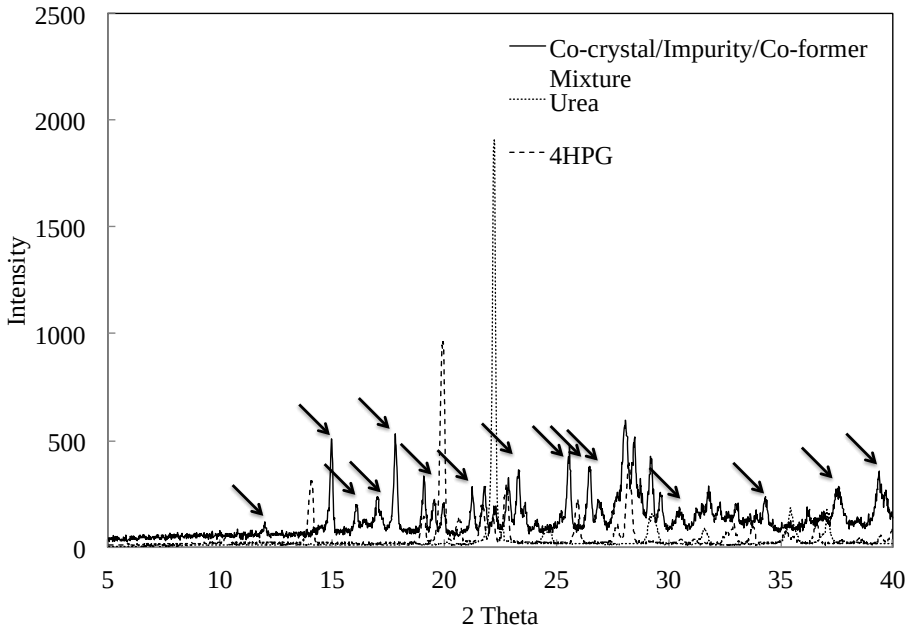


Figure 12 The Comparison between the Powder Pattern of the Cocrystal/4HPG/Urea Mixture and the Powder Patterns of the Individual Components.

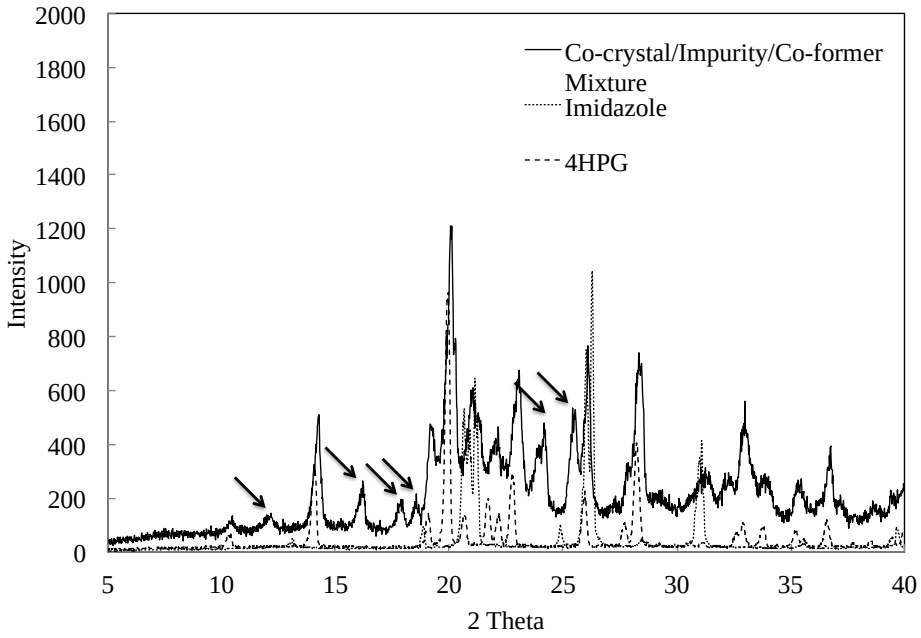


Figure 13 The Comparison between the Powder Pattern of the Cocrystal/4HPG/Imidazole Mixture and the Powder Patterns of the Individual Components.

3. Effect of Coformer Amount Added on the Amount of 4HPG Incorporated into AMCT Crystal Lattice.

Table 10. Effect of Coformer Amount Added on the Amount of 4HPG Incorporated into AMCT Crystal Lattice.

Coformer	Coformer-to-4HPG Molar Ratios (r)	Amount of 4HPG (%)	Decreased (%)
2-picolinic acid	0.1	0.92±0.01	6
	0.5	0.16±0.01	84
	1	0.17±0.01	83
	1.5	0.15±0.01	85
L-lysine	0.1	0.89±0.07	9
	0.5	0.15±0.01	85
	1	0.17±0.01	83
	1.5	0.18±0.01	82
L-leucine	0.1	0.87±0.06	11
	0.5	0.48±0.03	51
	1	0.12±0.01	88
	1.5	0.13±0.01	87
L-isoleucine	0.1	0.79±0.08	19
	0.5	0.42±0.03	57
	1	0.15±0.01	85
	1.5	0.12±0.01	88