An *ab initio* molecular dynamics method for cocrystal prediction: A validation of the approach

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Electronic Supporting Information

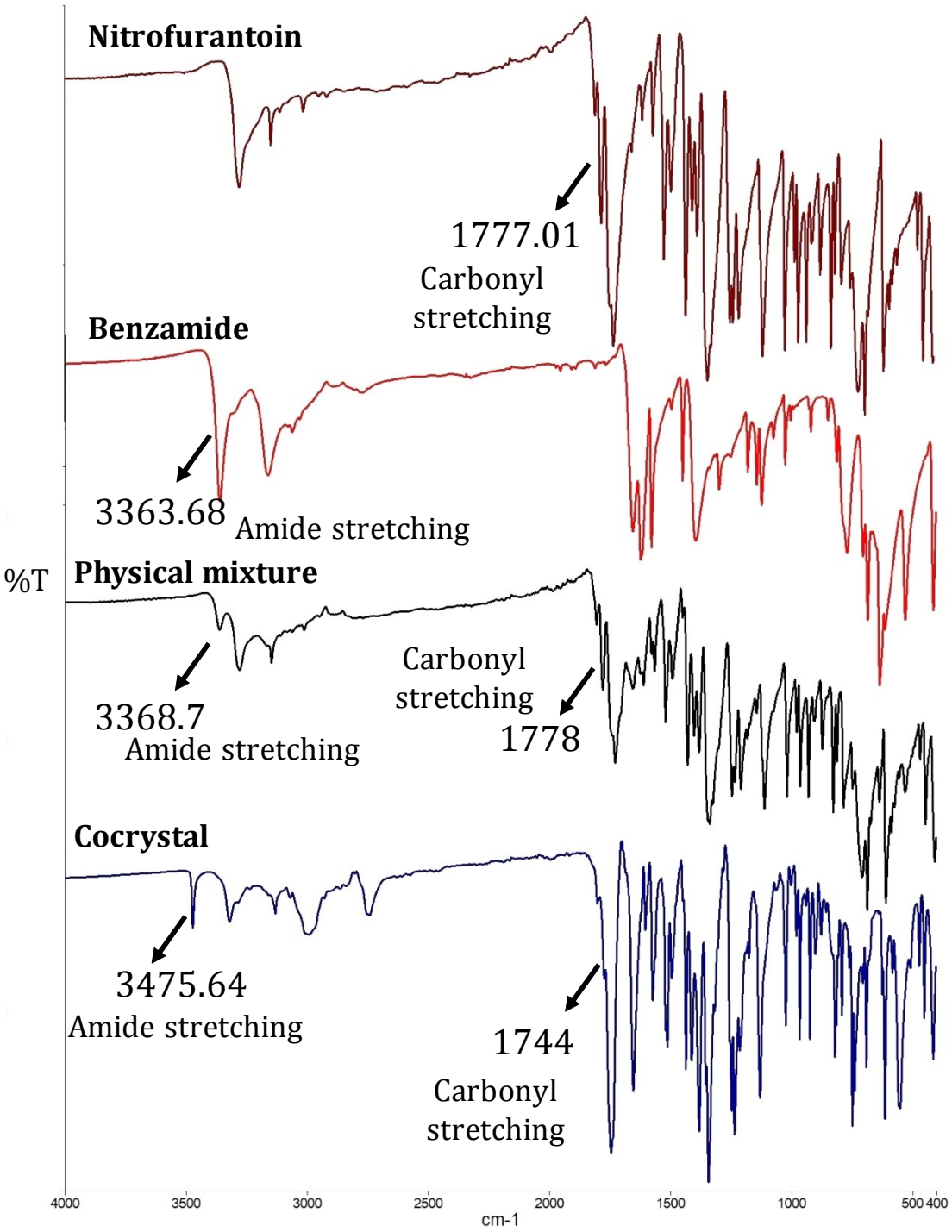


Figure S1: Infrared spectrum overlay for nitrofurantoin-benzamide cocrystal

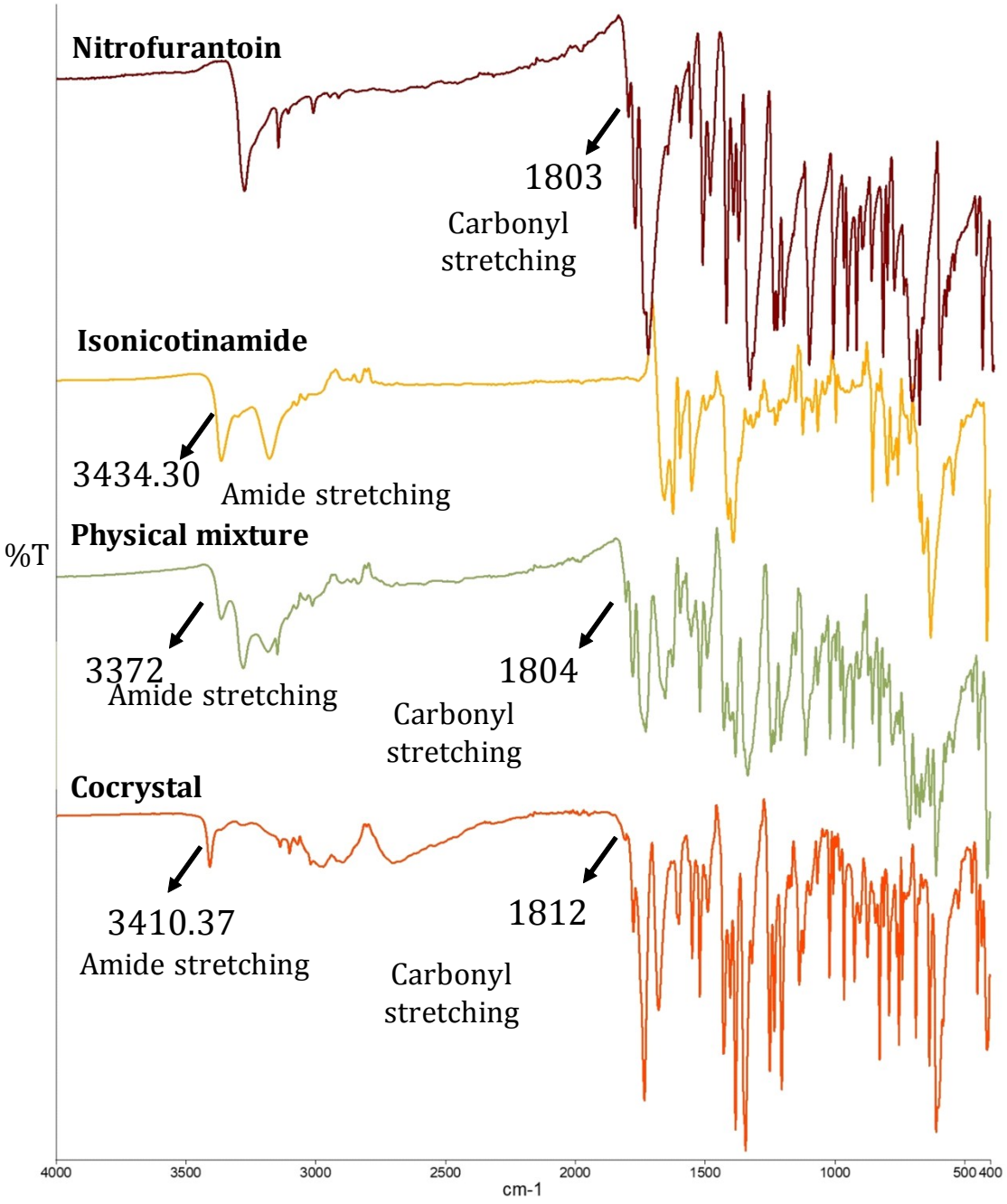


Figure S2: Infrared spectrum overlay for nitrofurantoin-isonicotinamide cocrystal

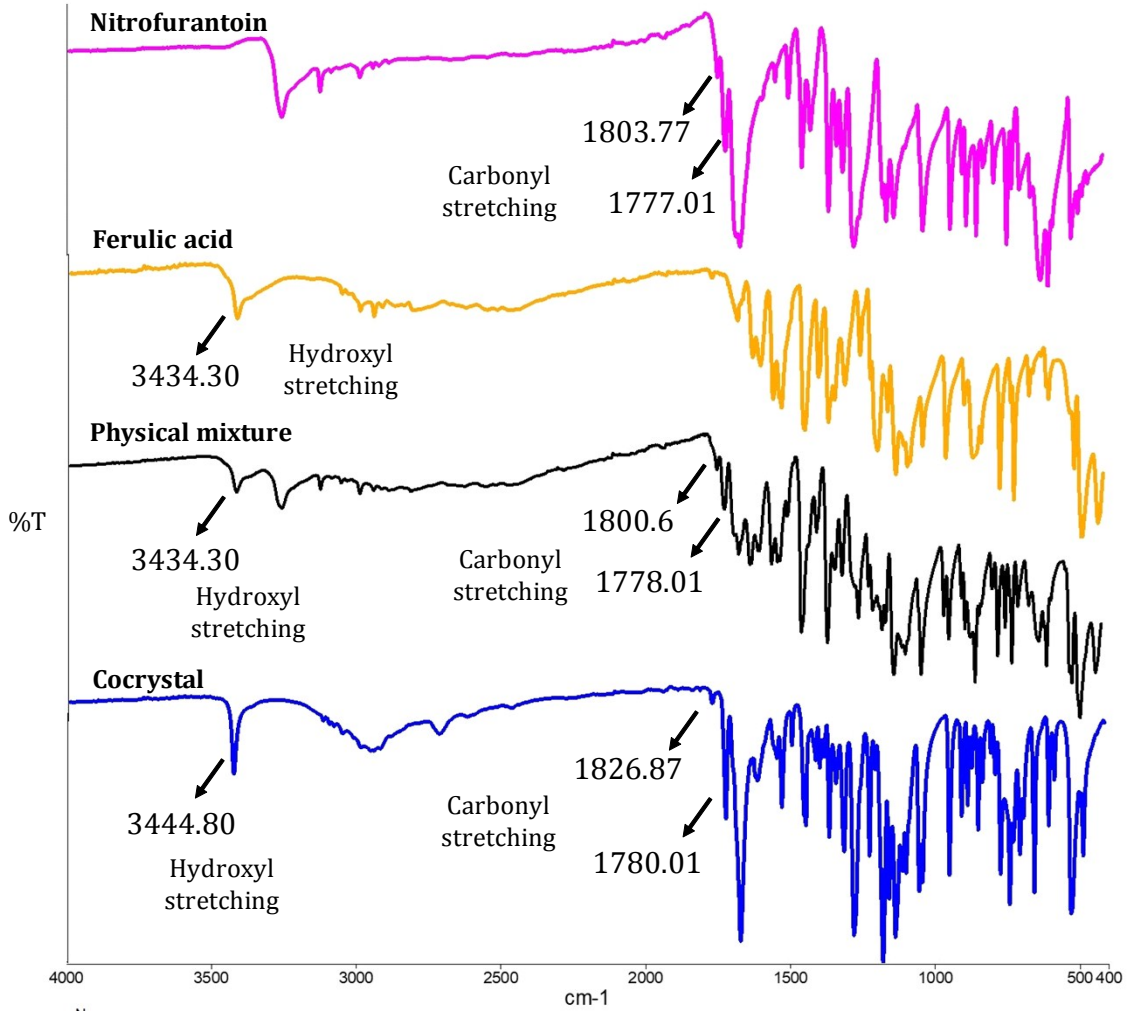


Figure S3: Infrared spectrum overlay for nitrofurantoin-ferulic acid cocrystal

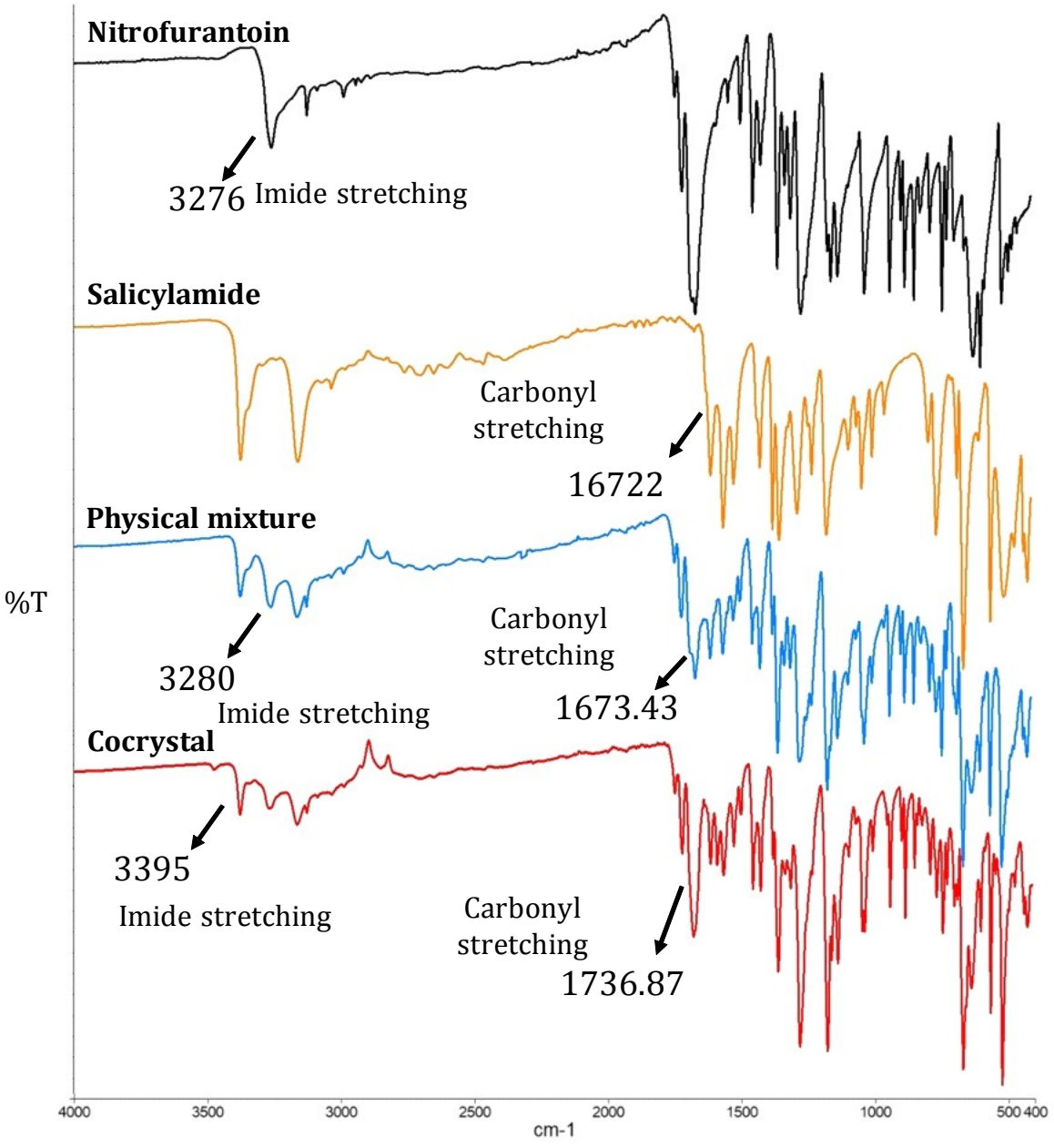
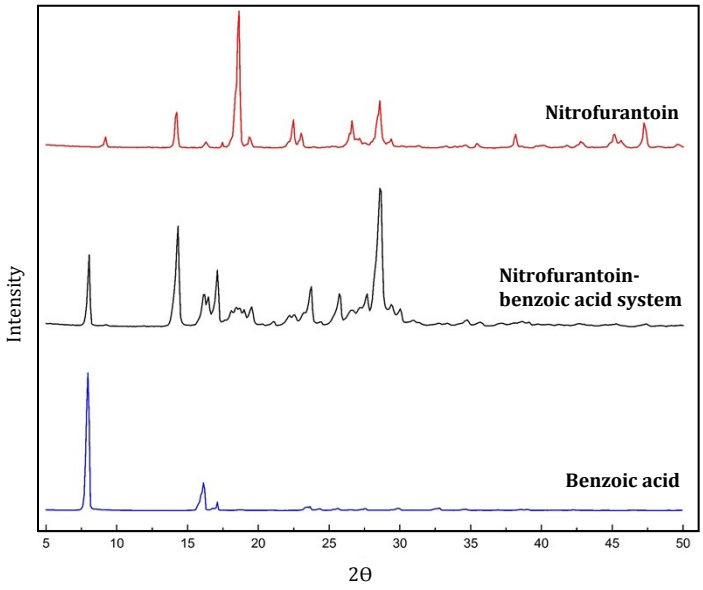
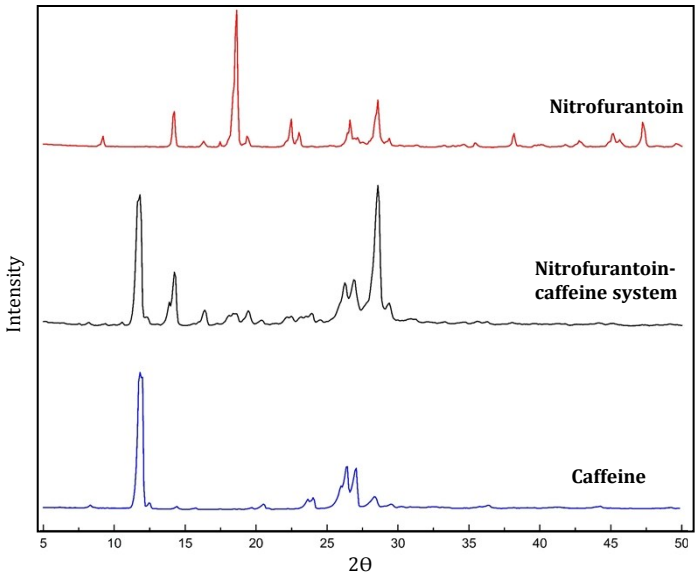
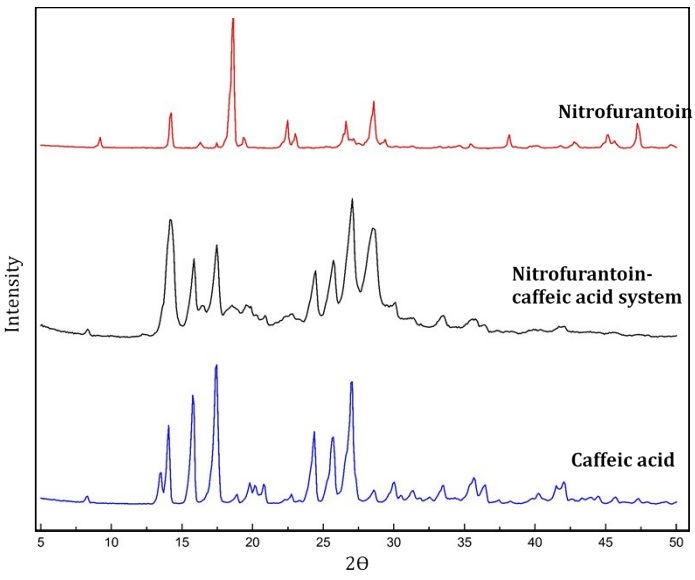
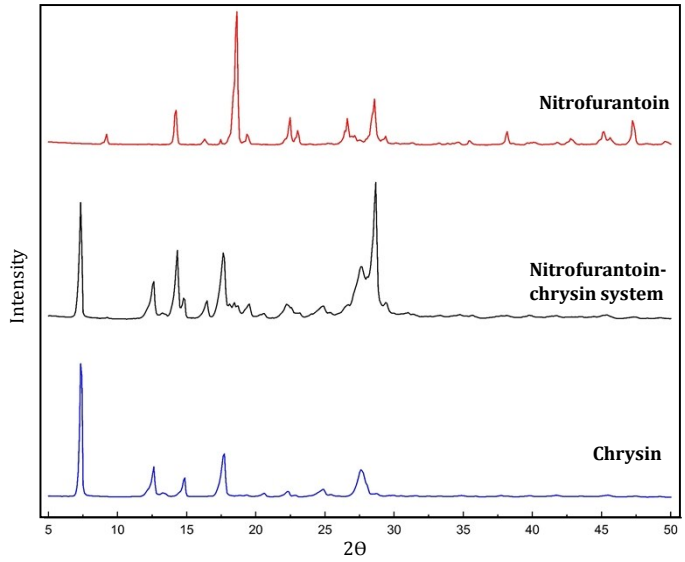


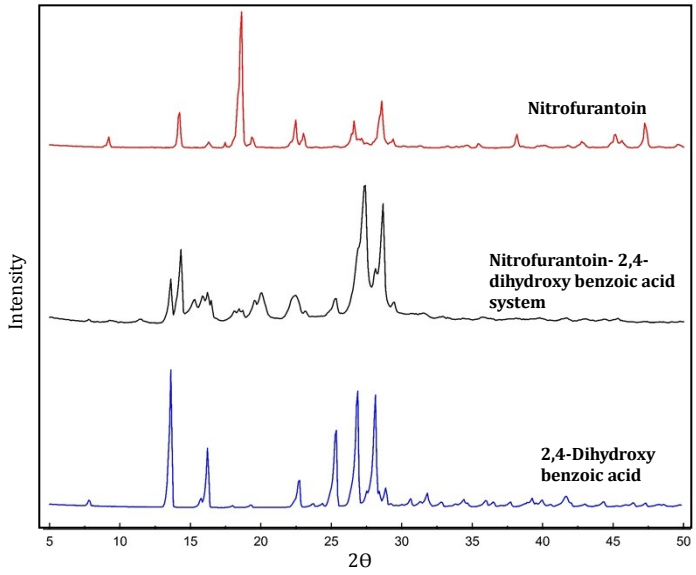
Figure S4: Infrared spectrum overlay for nitrofurantoin-salicylamide cocrystal

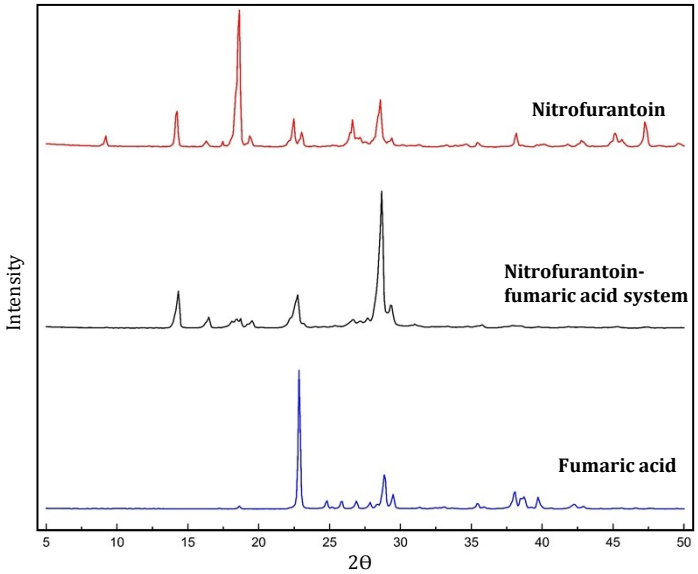

Nitrofurantoin
Nitrofurantoin-
benzoic acid system
Benzoic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

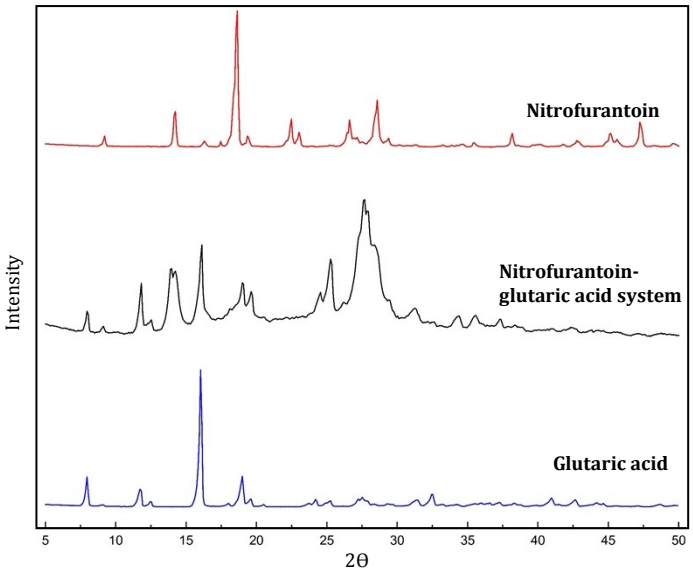

Nitrofurantoin
Nitrofurantoin-
caffeine system
Caffeine
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

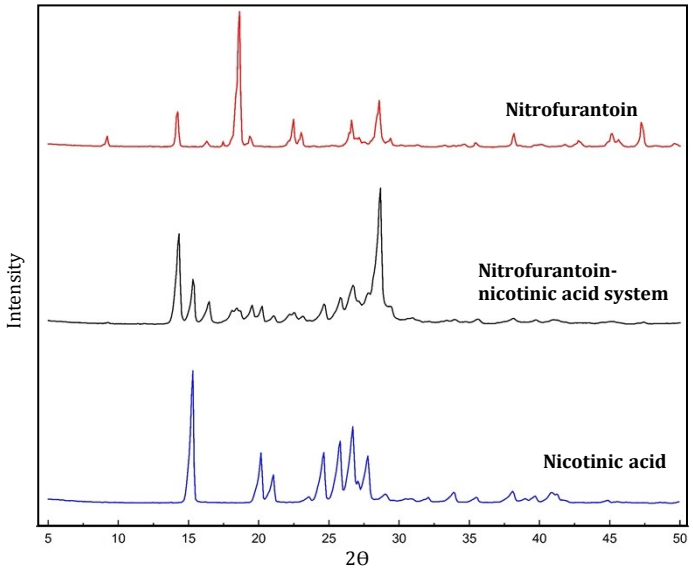

Nitrofurantoin
Nitrofurantoin-
caffeic acid system
Caffeic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

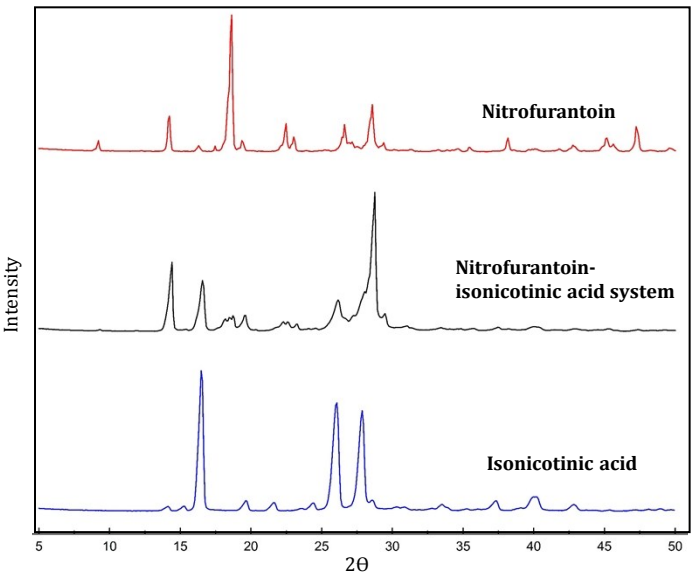

Nitrofurantoin
Nitrofurantoin-
chrysin system
Chrysin
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

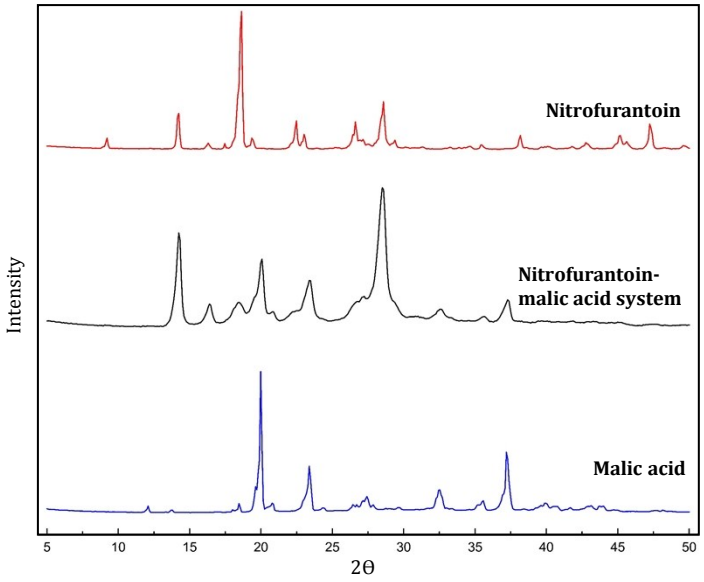

Nitrofurantoin
Nitrofurantoin- 2,4-
dihydroxy benzoic acid
system
2,4-Dihydroxy
benzoic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

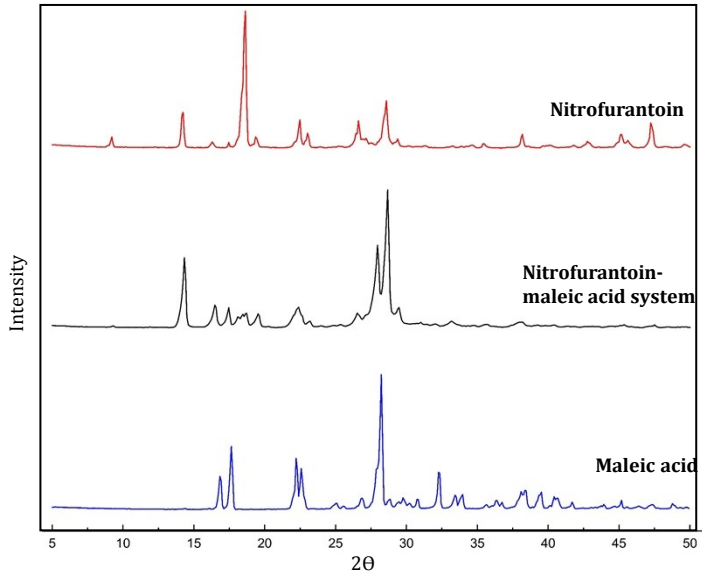

Nitrofurantoin
Nitrofurantoin-
fumaric acid system
Fumaric acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

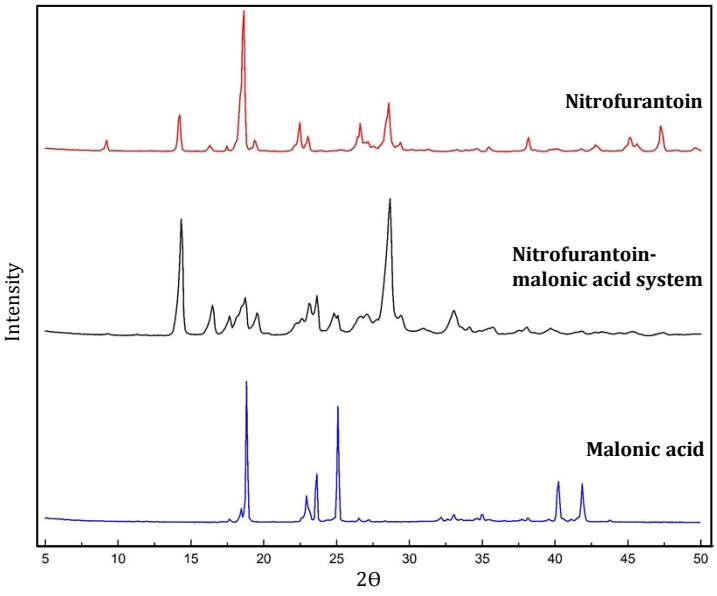

Nitrofurantoin
Nitrofurantoin-
glutaric acid system
Glutaric acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

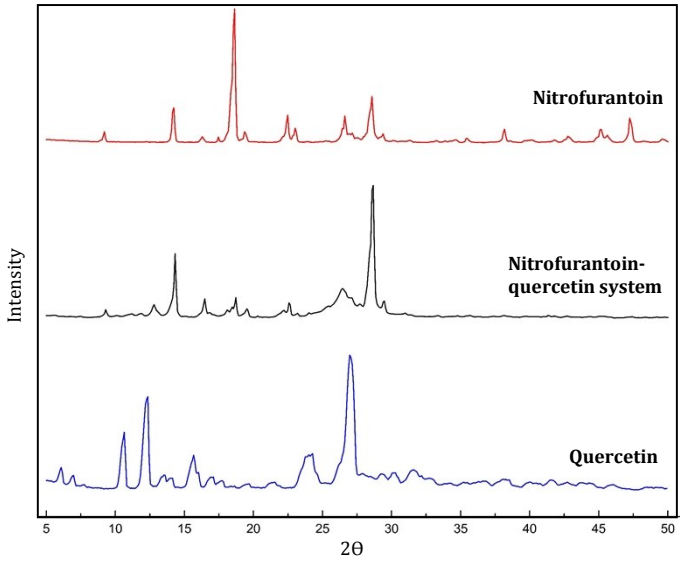

Nitrofurantoin
Nitrofurantoin-
nicotinic acid system
Nicotinic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

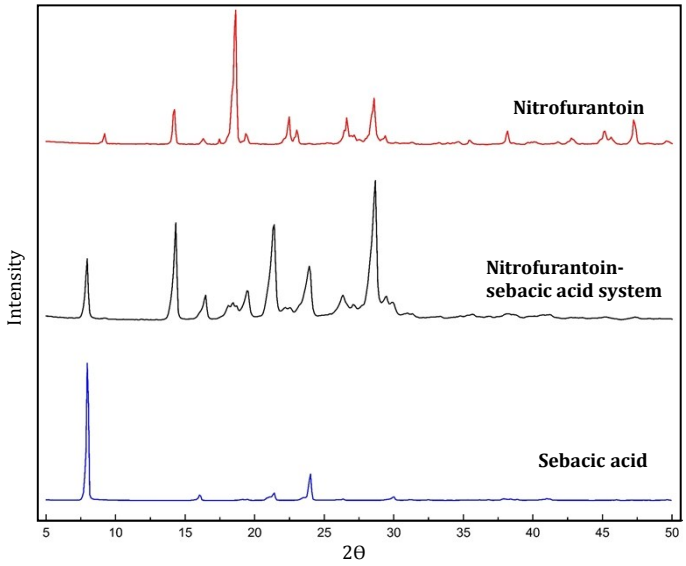

Nitrofurantoin
Nitrofurantoin-
isonicotinic acid system
Isonicotinic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

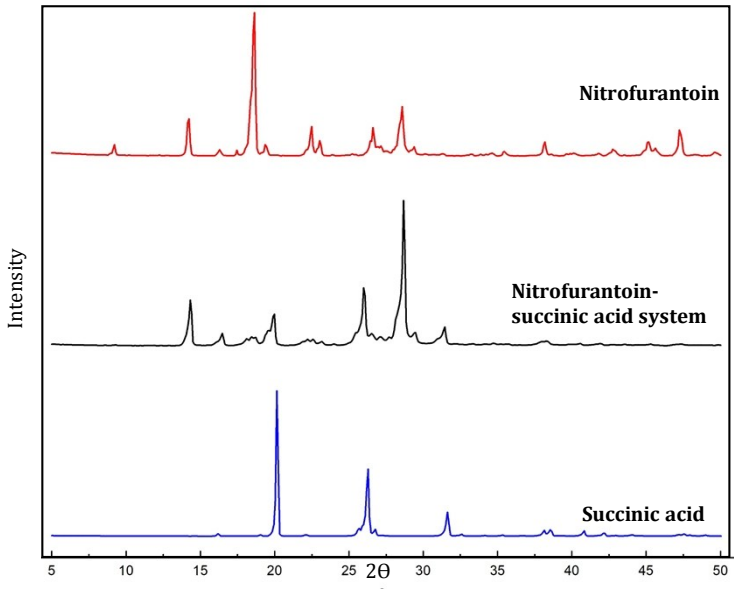

Nitrofurantoin
Nitrofurantoin-
malic acid system
Malic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

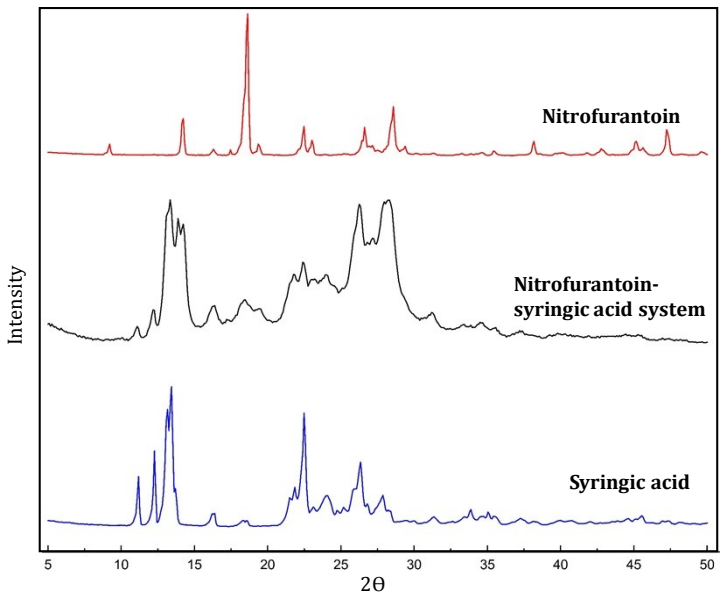

Nitrofurantoin
Nitrofurantoin-
maleic acid system
Maleic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ


Nitrofurantoin
Nitrofurantoin-
malonic acid system
Malonic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ


Nitrofurantoin
Nitrofurantoin-
quercetin system
Quercetin
Intensity
5
10
15
20
25
30
35
40
45
50
2θ


Nitrofurantoin
Nitrofurantoin-
sebacic acid system
Sebacic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ


Nitrofurantoin
Nitrofurantoin-
succinic acid system
Succinic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ


Nitrofurantoin
Nitrofurantoin-
syringic acid system
Syringic acid
Intensity
5
10
15
20
25
30
35
40
45
50
2θ

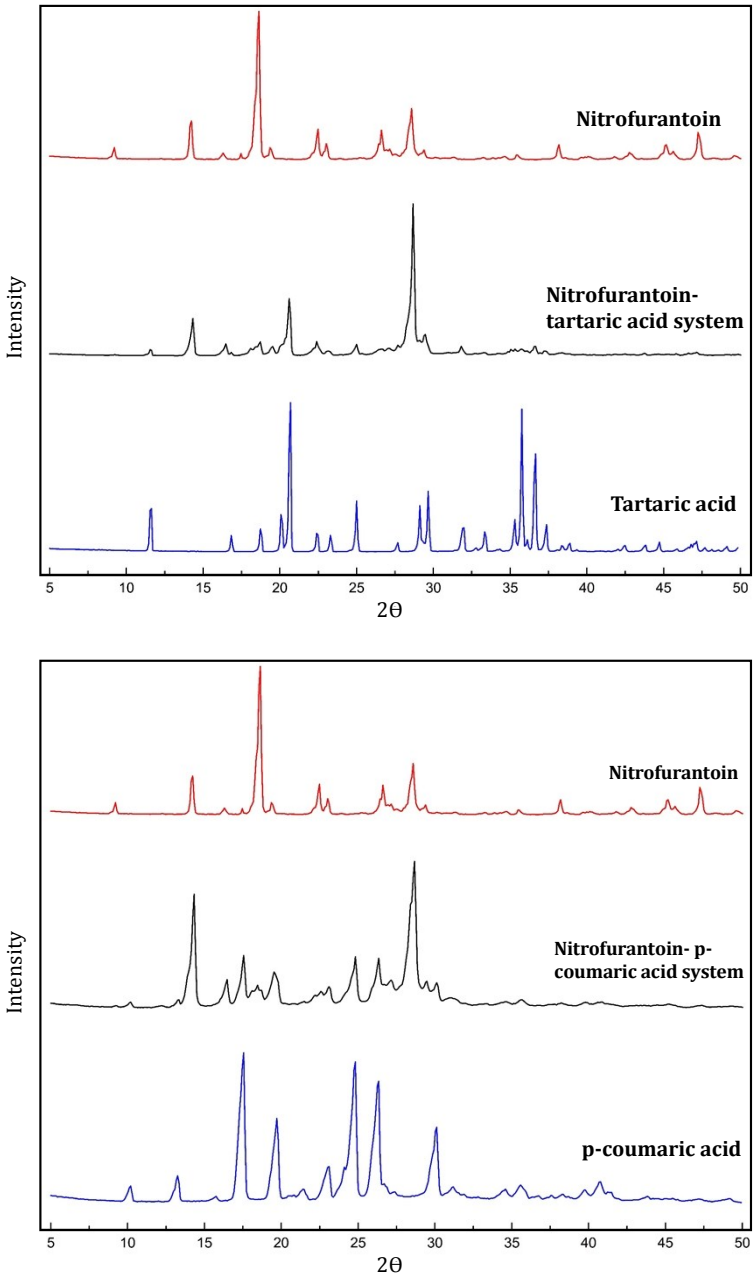


Figure S5: Powder X-ray diffraction overlay for generated cogrinded samples with nitrofurantoin and respective coformer