Supplementary Materials: Application of 1-Hydroxy-4,5-Dimethyl-Imidazole 3-Oxide as Coformer in Formation of Pharmaceutical Cocrystals

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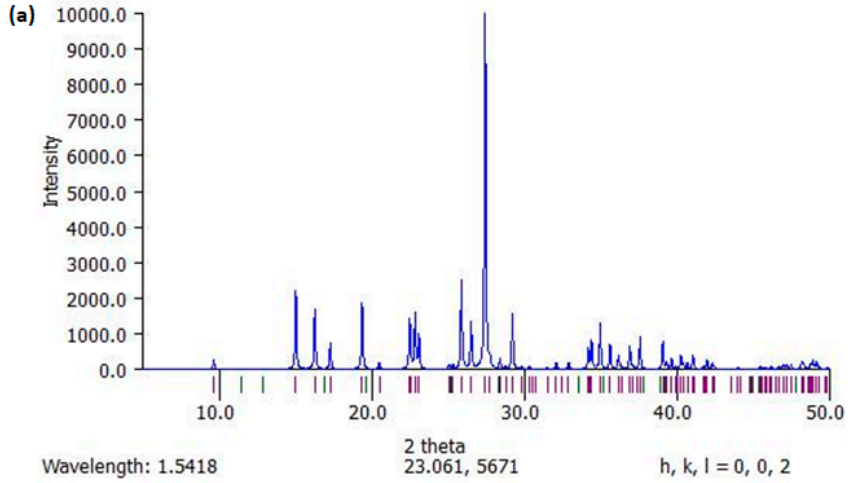
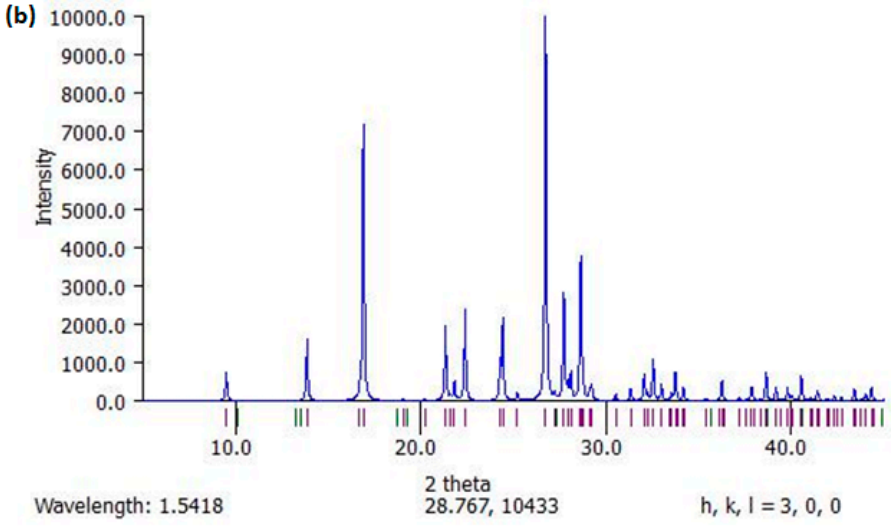




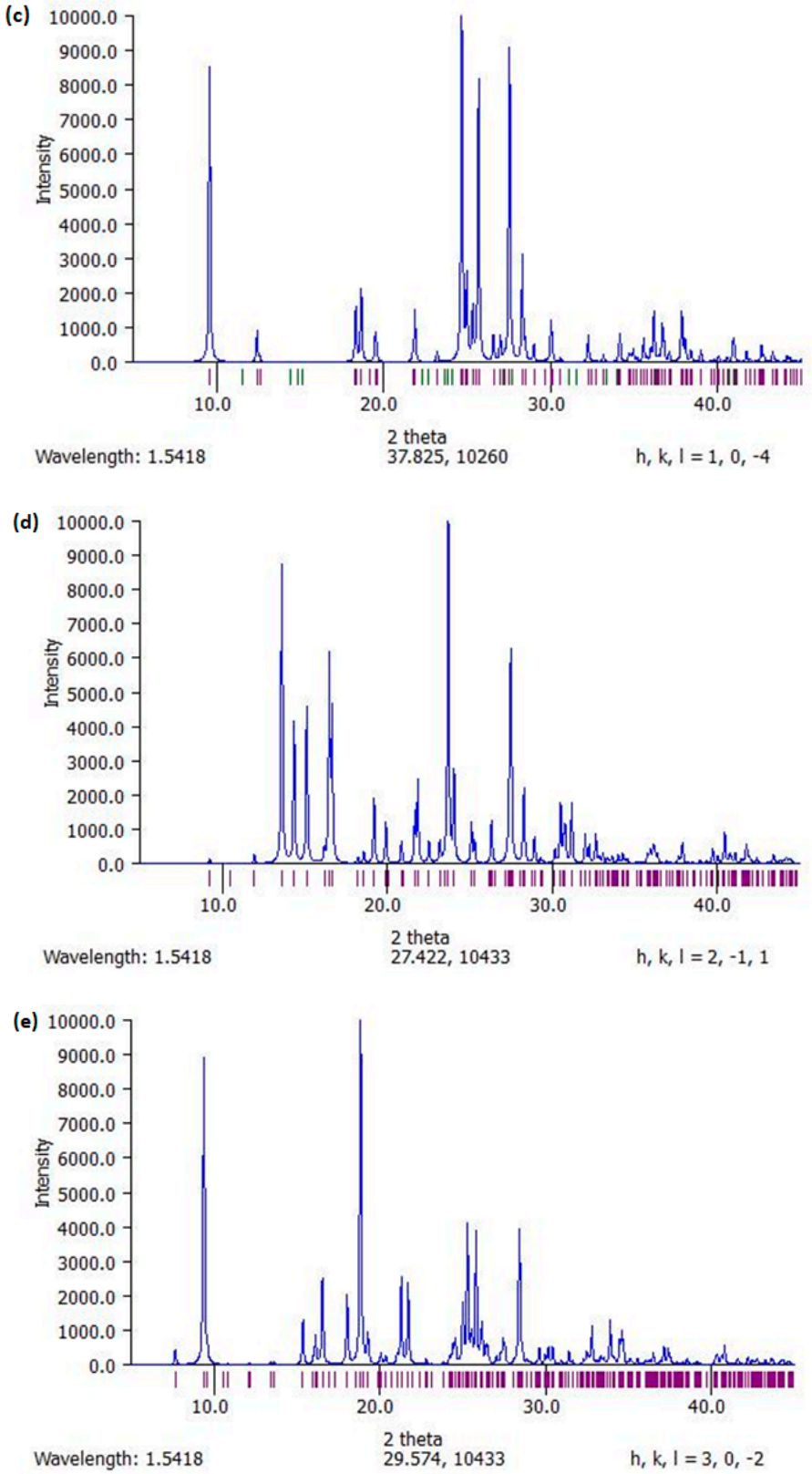


Figure S1. Calculated powder x-ray diffraction diffractograms (from top to bottom) TBA crystallized from acetonitryl (tautomer A)[1]; TBA crystallized from ethanol (tautomer B)[1]; TBA crystallized from water (tautomer B)[1]; HIMO; TBA/HIMO.

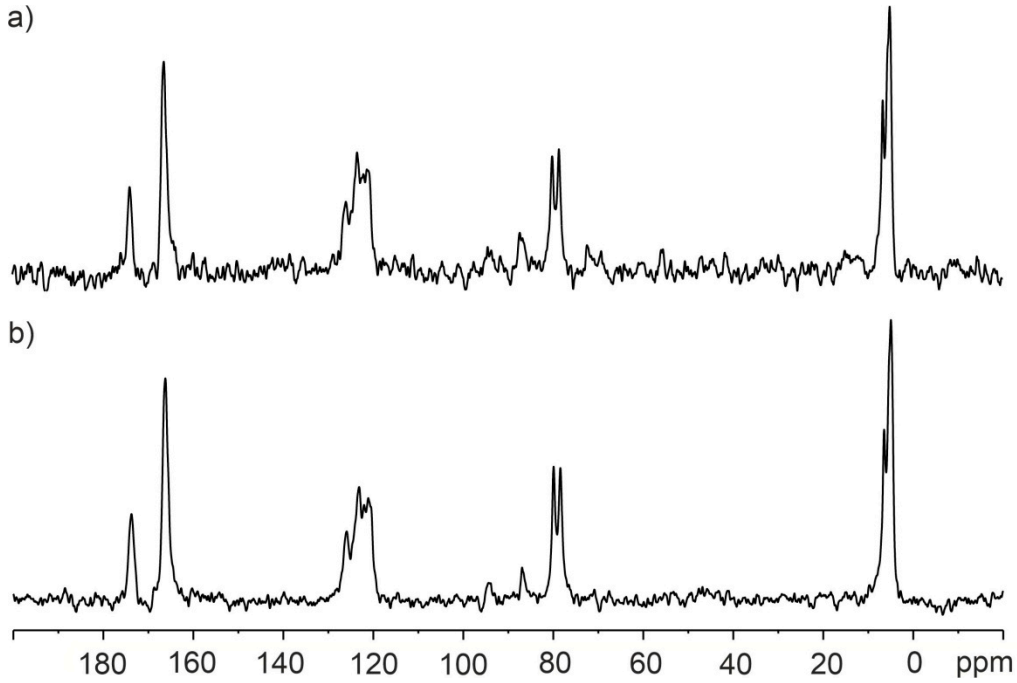
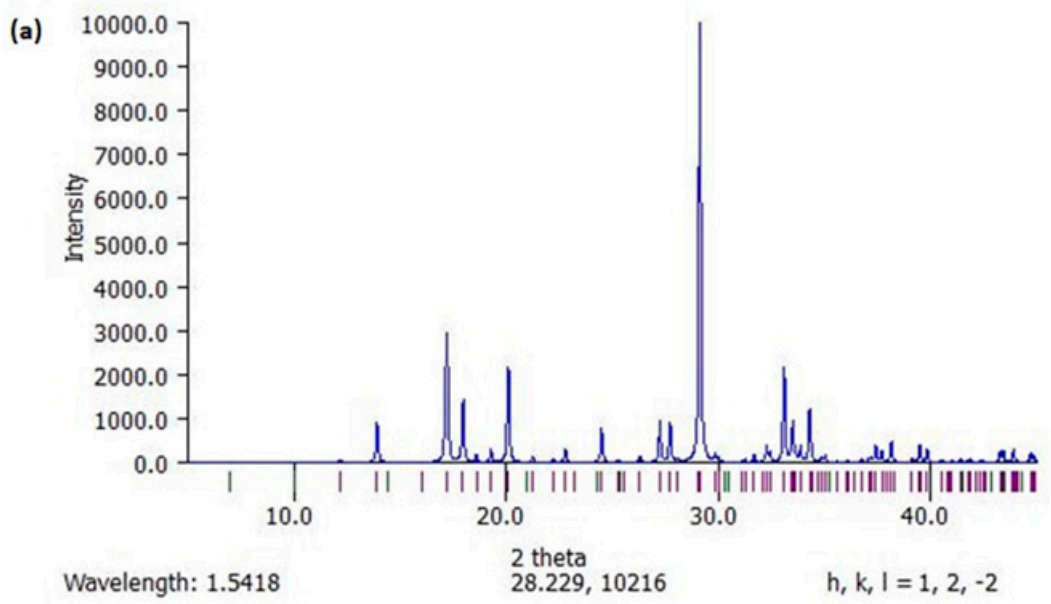
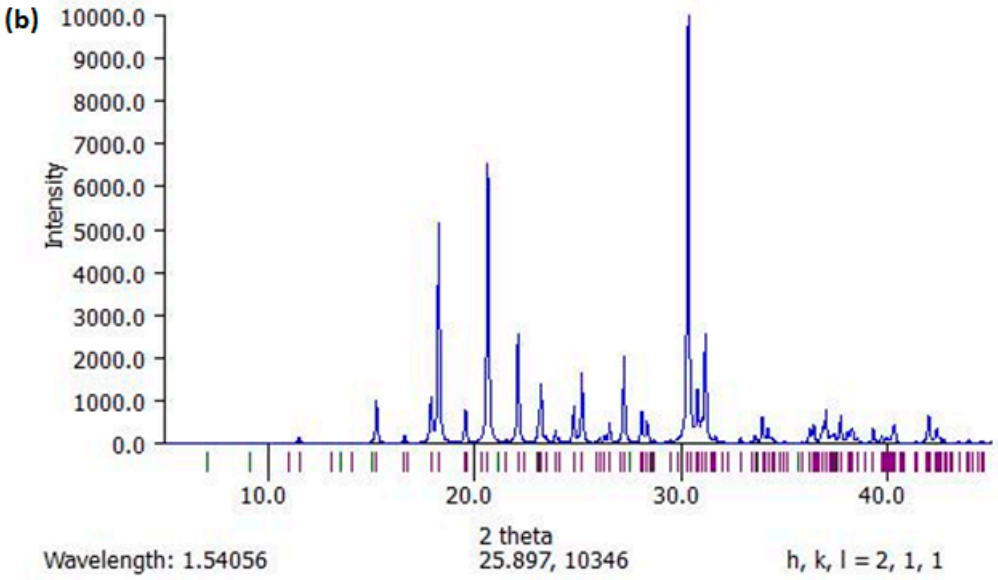
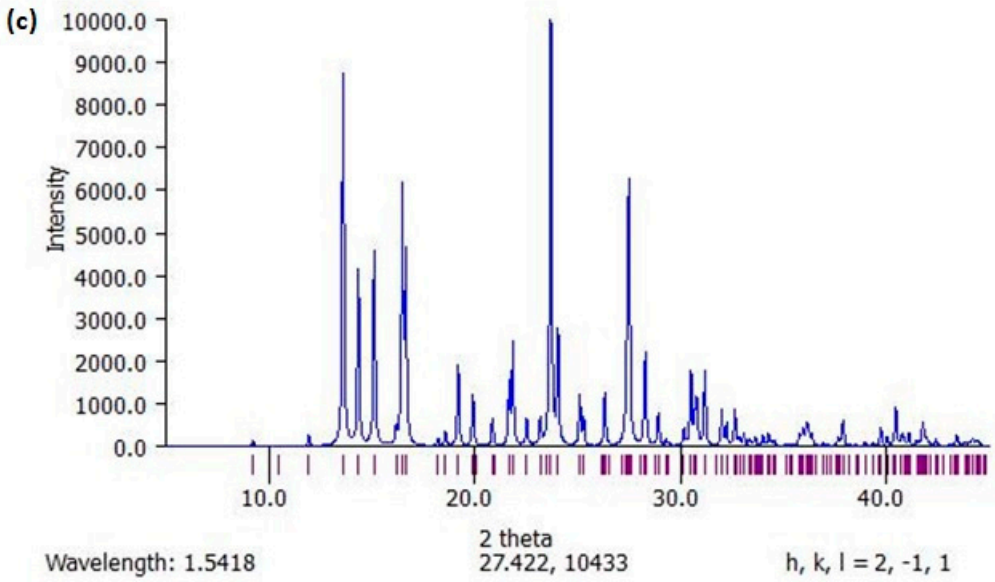


Figure S2. ^{13}C CP/MAS spectra recorded with a spinning rate of 8 kHz for TBA/HIMO cocrystals obtained by (**a**) grinding; (**b**) cocrystallization from MeOH.




(b)
10000.0
9000.0
8000.0
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
Intensity
10.0
20.0
30.0
40.0
2 theta
Wavelength: 1.54056
25.897, 10346
h, k, l = 2, 1, 1


(c)
10000.0
9000.0
8000.0
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
Intensity
10.0
20.0
30.0
40.0
2 theta
Wavelength: 1.5418
27.422, 10433
h, k, l = 2, -1, 1

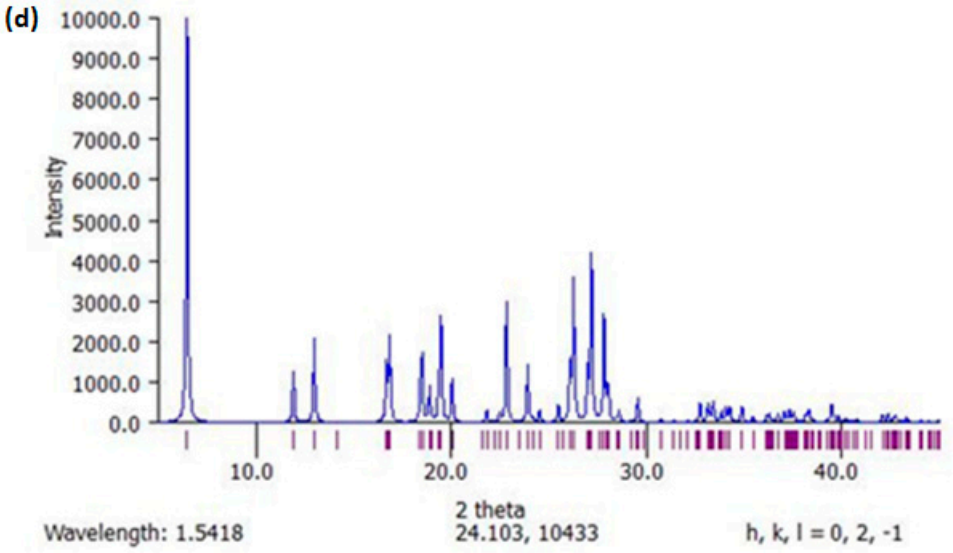

(d)
10000.0
9000.0
8000.0
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
Intensity
10.0
20.0
30.0
40.0
2 theta
Wavelength: 1.5418
24.103, 10433
h, k, l = 0, 2, -1

Figure S3. Calculated powder x-ray diffraction diffractograms (from top to bottom) for; BA (form II)[2], BA dihydrate[3]; HIMO and BA/HIMO.

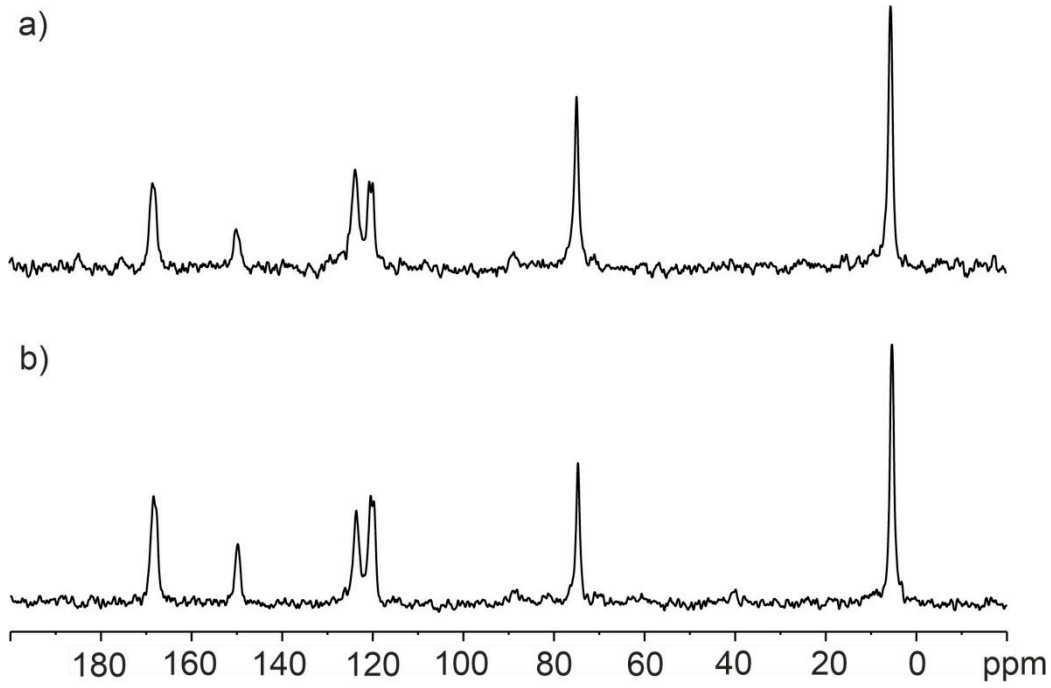


Figure S4. ^{13}C CP/MAS spectra recorded with a spinning rate of 8 kHz for BA/HIMO cocrystals obtained by (**a**) grinding; (**b**) cocrystallization from MeOH.

References

1. Chierotti, M.R.; Ferrero, L.; Garino, N.; Gobetto, R.; Pellegrino, L.; Braga, D.; Grepioni, F.; Maini, L. The Richest Collection of Tautomeric Polymorphs: The Case of 2-Thiobarbituric Acid. *Chem. Eur. J.* **2010**, *16*, 4347–4358.
2. Lewis T. C, Tocher D. A., Price S. L. An Experimental and Theoretical Search for Polymorphs of Barbituric Acid: The Challenges of Even Limited Conformational Flexibility Crystal Growth & Design **2004**, *4*, 979-987
3. Nichol G.S., Clegg W., *Acta Crystallographica,Section B: Structural Science*, A variable-temperature study of a phase transition in barbituric acid dihydrate **2005**, *61*, 464-472