Electronic Supplementary Material (ESI) for CrystEngComm

Mechanochemical Synthesis of Pyrazine:Dicarboxylic Acid Cocrystals and the study of their Dissociation by Quantitative Phase Analysis

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Supplementary Information

Table S1. Theoretical and experimental weight loss determined by TGA of the pyrazine cocrystals.

Cocrystal	Weight loss (experimental) / %	Weight loss (theoretical) / %
pyrazine:terephthalic	30.0	32.5
pyrazine:phthalic	31.4	32.5
pyrazine:succinic	40.0	40.4
pyrazine:fumaric	39.6	40.8

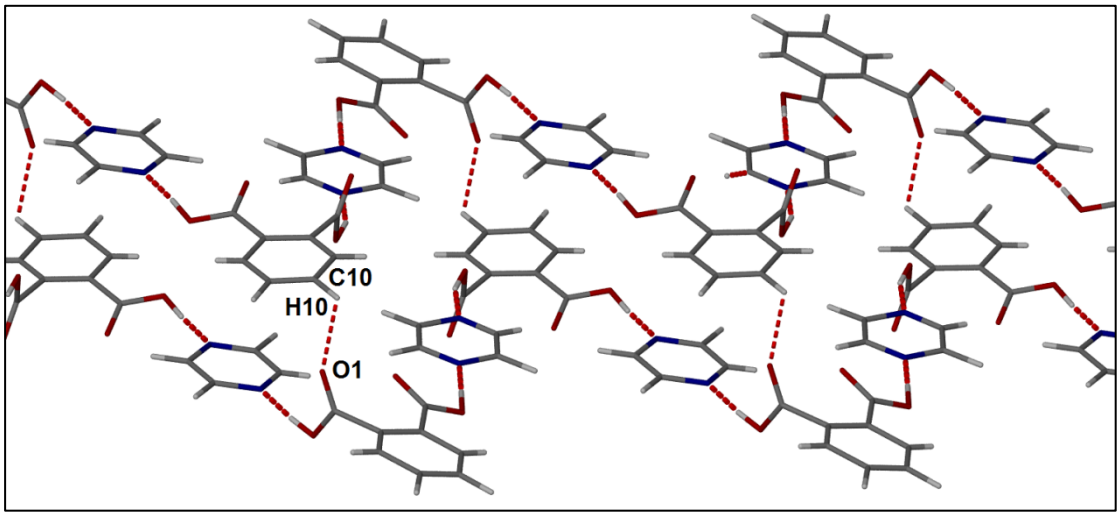

Figure S1. Close contact between atoms H10 and O1 (*x, 3/2-y, ½+z*) in the **pyr:pht** crystal structure.

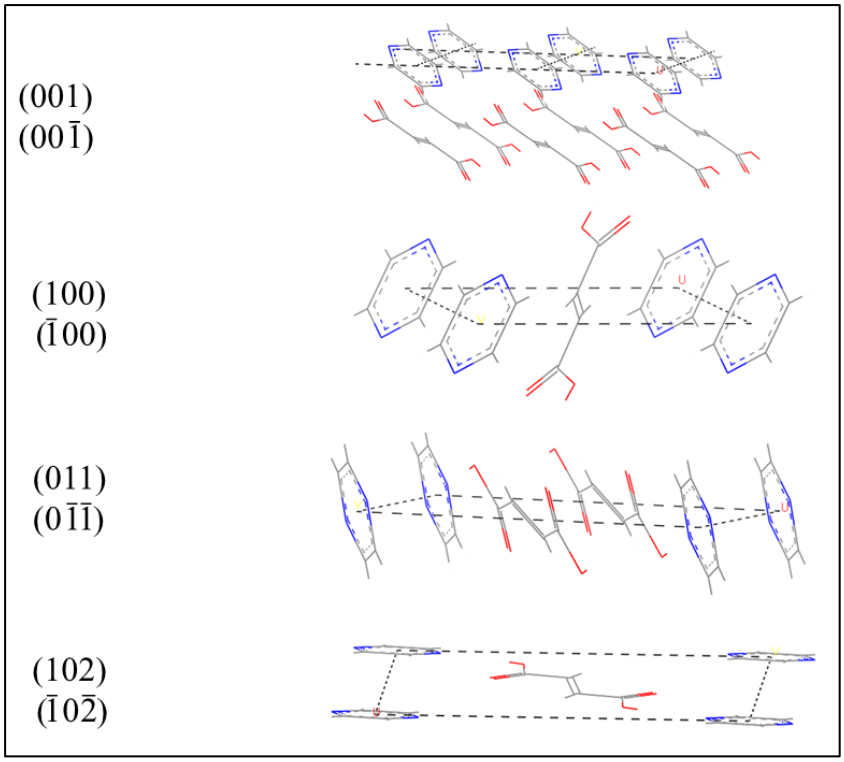

Figure S2. Molecular arrangements of the **pyr:fum** crystal faces. Faces (001) and (100) display hydrophilic character while faces (011) and (102) are mostly hydrophobic.

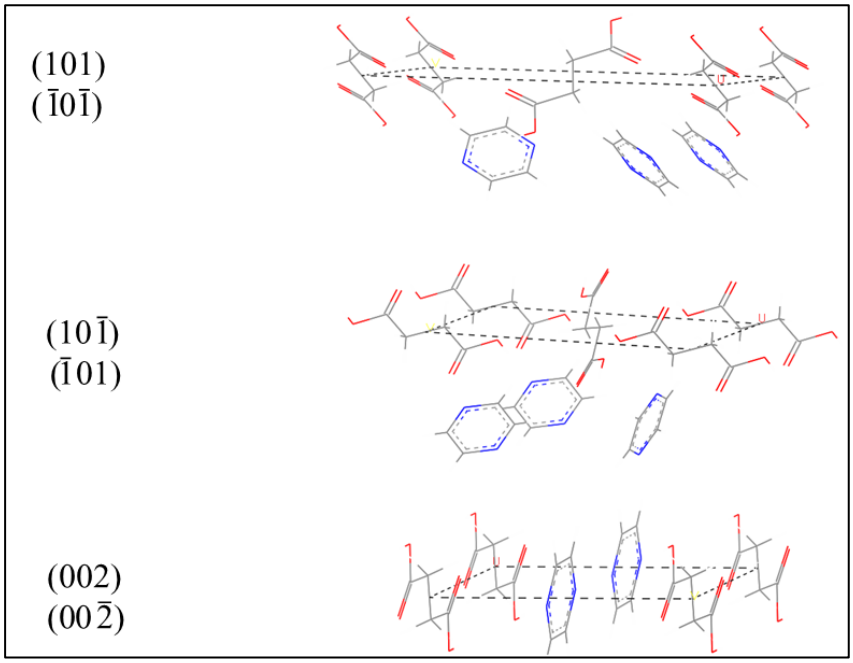

Figure S3. Molecular arrangements of the **pyr:succ** crystal faces. Faces (101) (10$\bar{1}$) and (002) are hydrophilic.

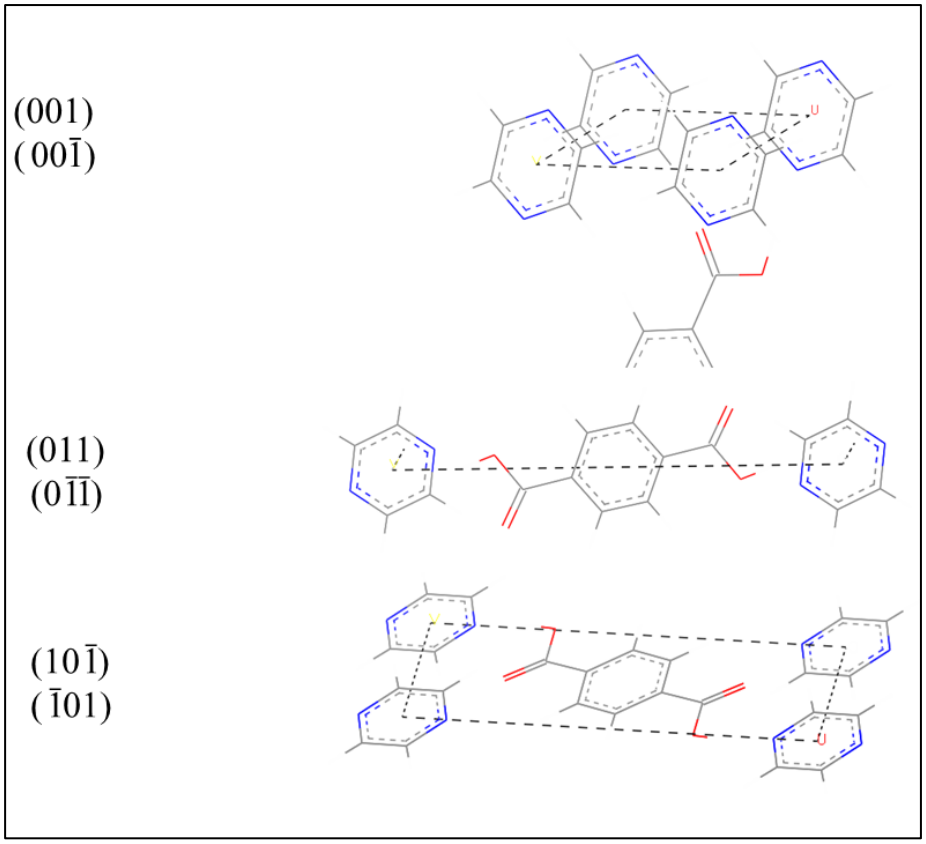

Figure S4. Molecular arrangements of the **pyr:ter** crystal faces. (001) face is hydrophilic while (011) and (10$\bar{1}$) faces are mostly hydrophobic.

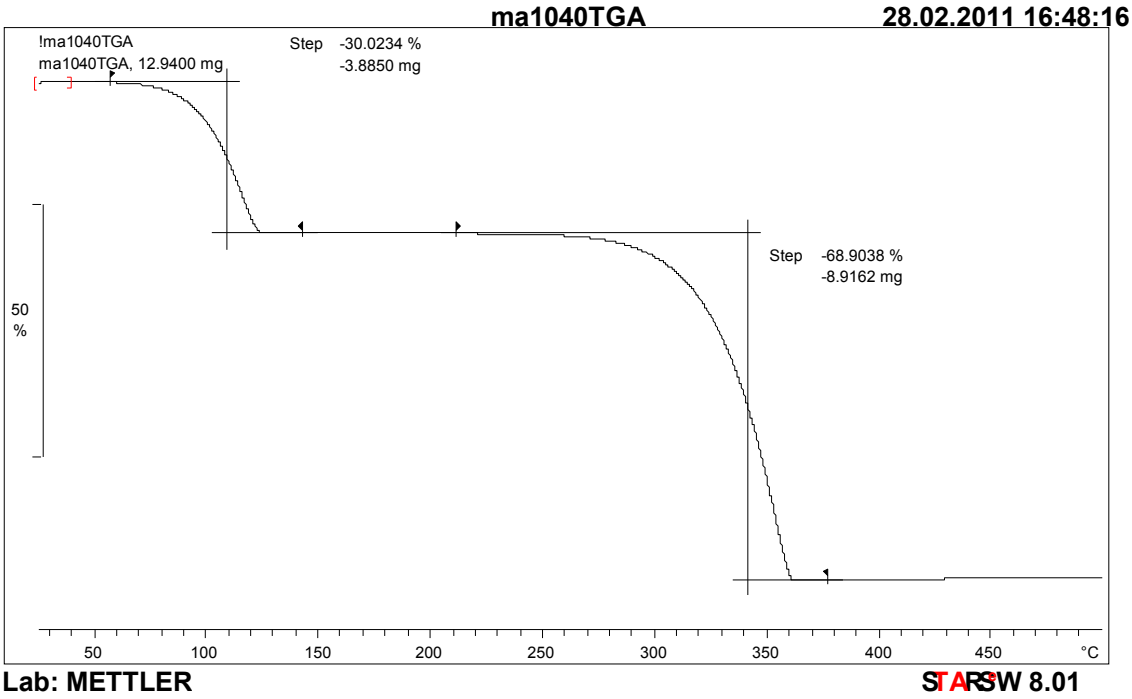

Figure S5. TGA of pyrazine:terephthalic acid cocrystal

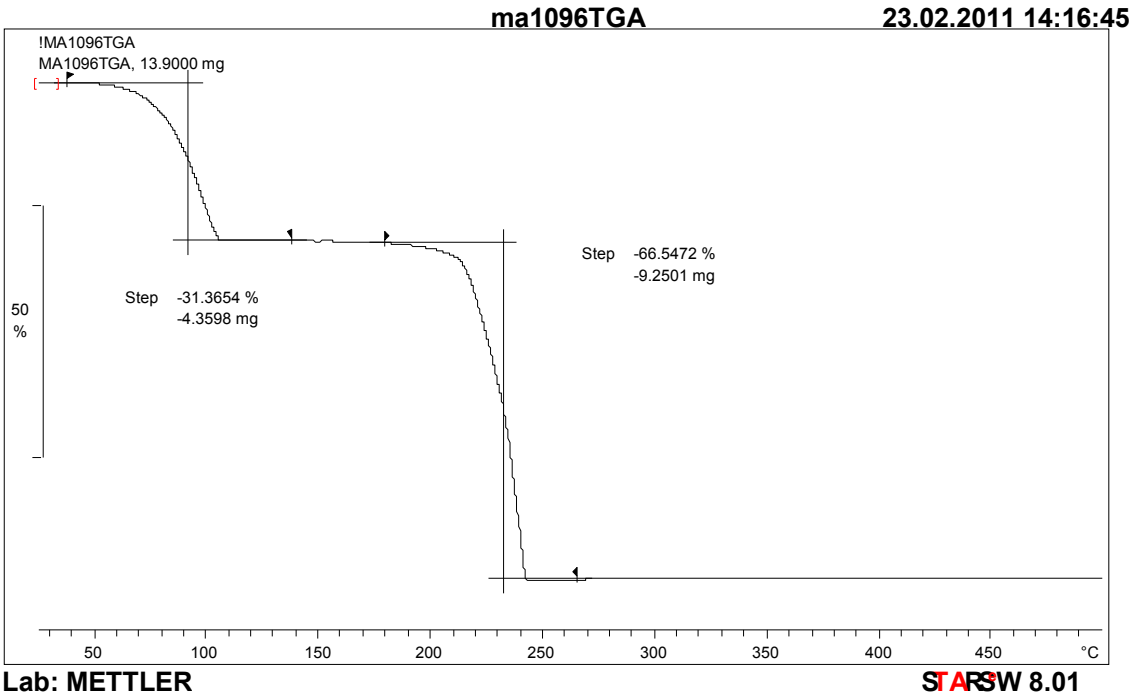

Figure S6. TGA of pyrazine:phthalic acid cocrystal

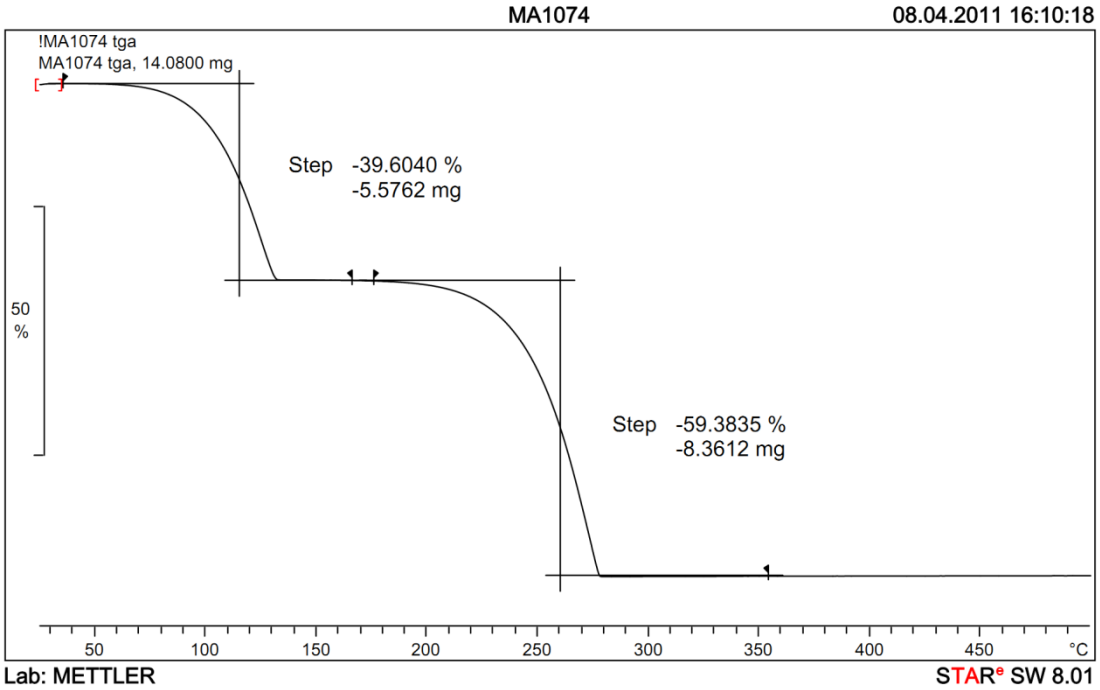

Figure S7. TGA of pyrazine:fumaric acid cocrystal

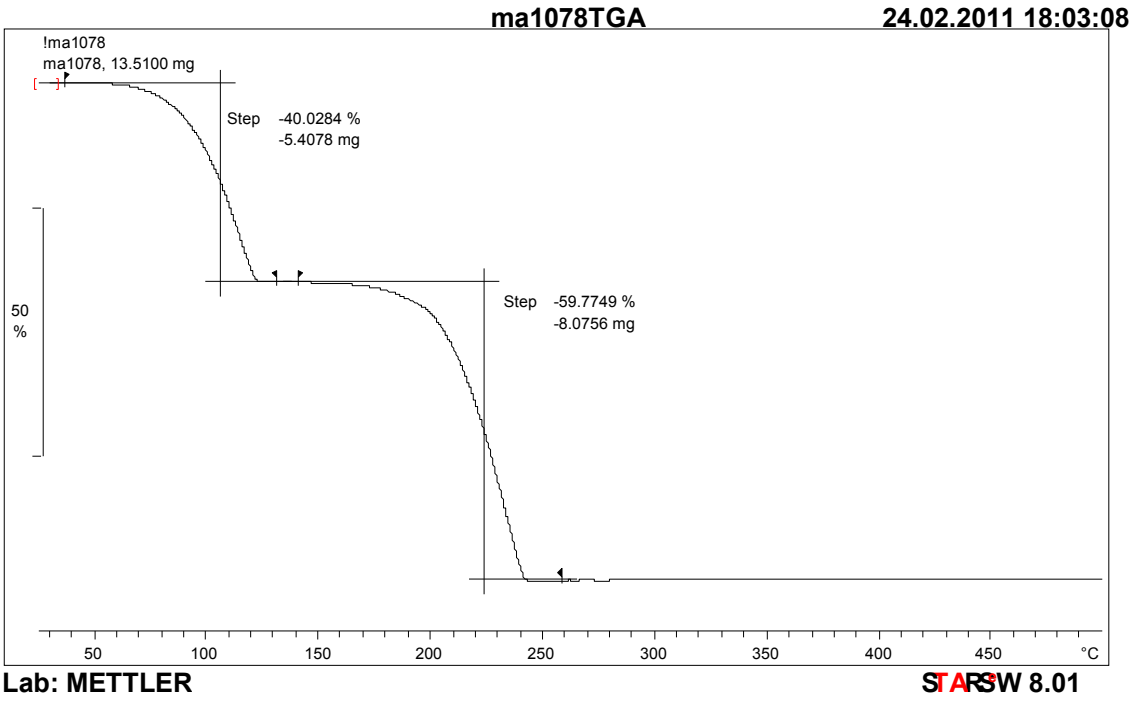

Figure S8. TGA of pyrazine:succinic acid cocrystal

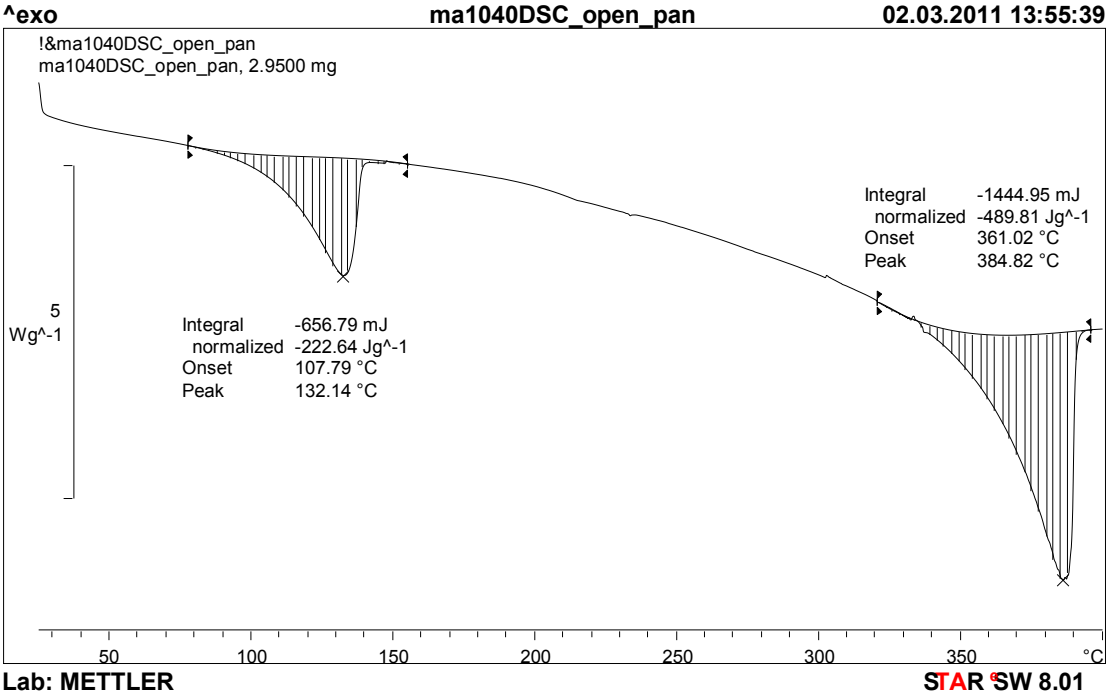

Figure S9. DSC of pyrazine:terephthalic acid cocrystal

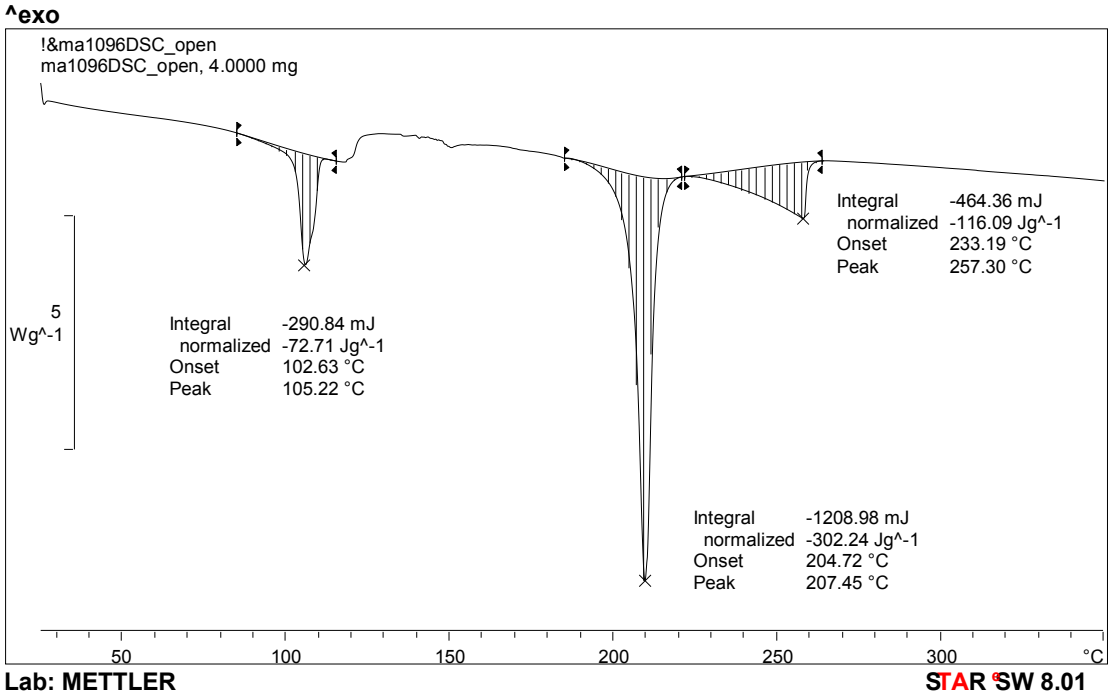

Figure S10. DSC of pyrazine:phthalic acid cocrystal

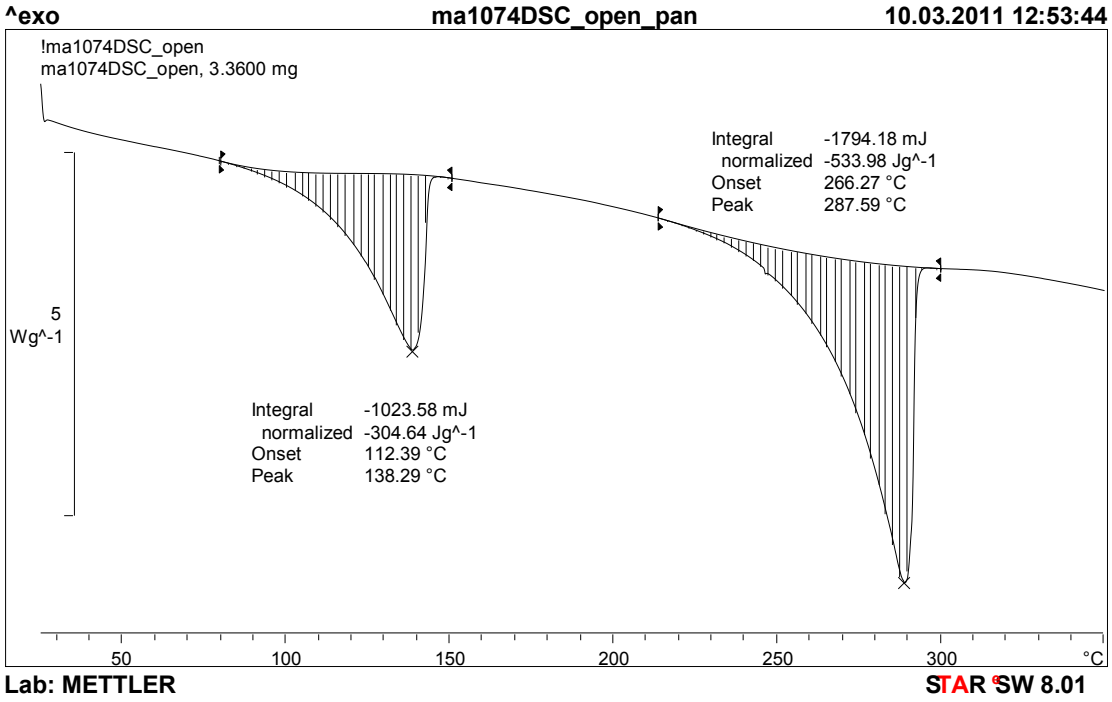

Figure S11. DSC of pyrazine:fumaric acid cocrystal

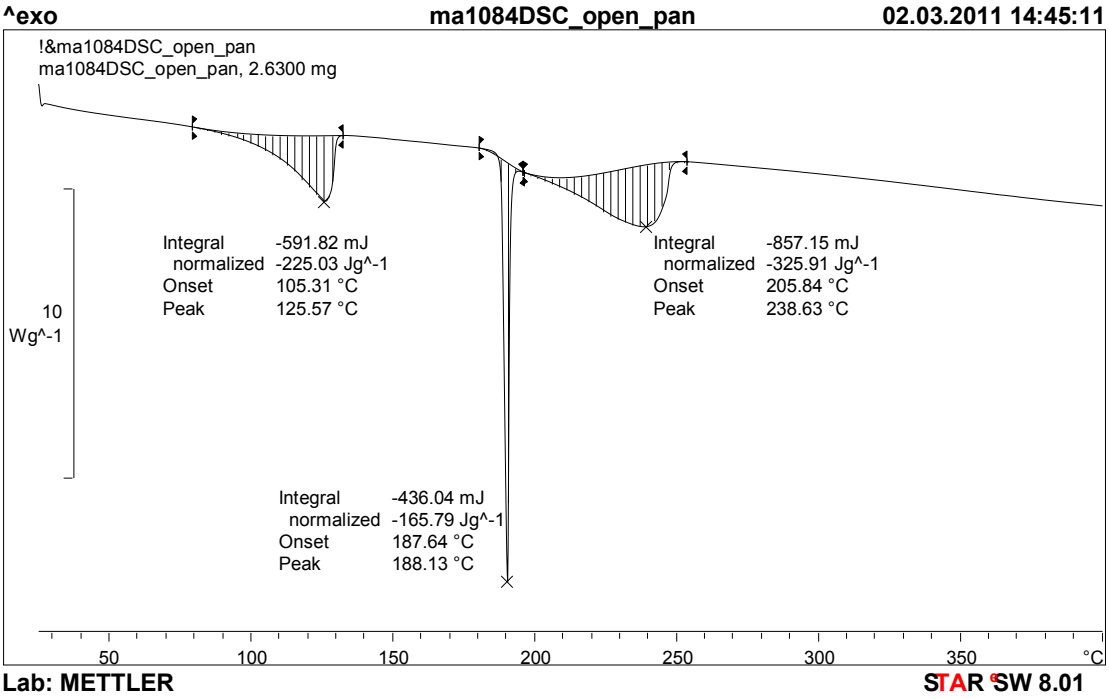

Figure S12. DSC of pyrazine:succinic acid cocrystal

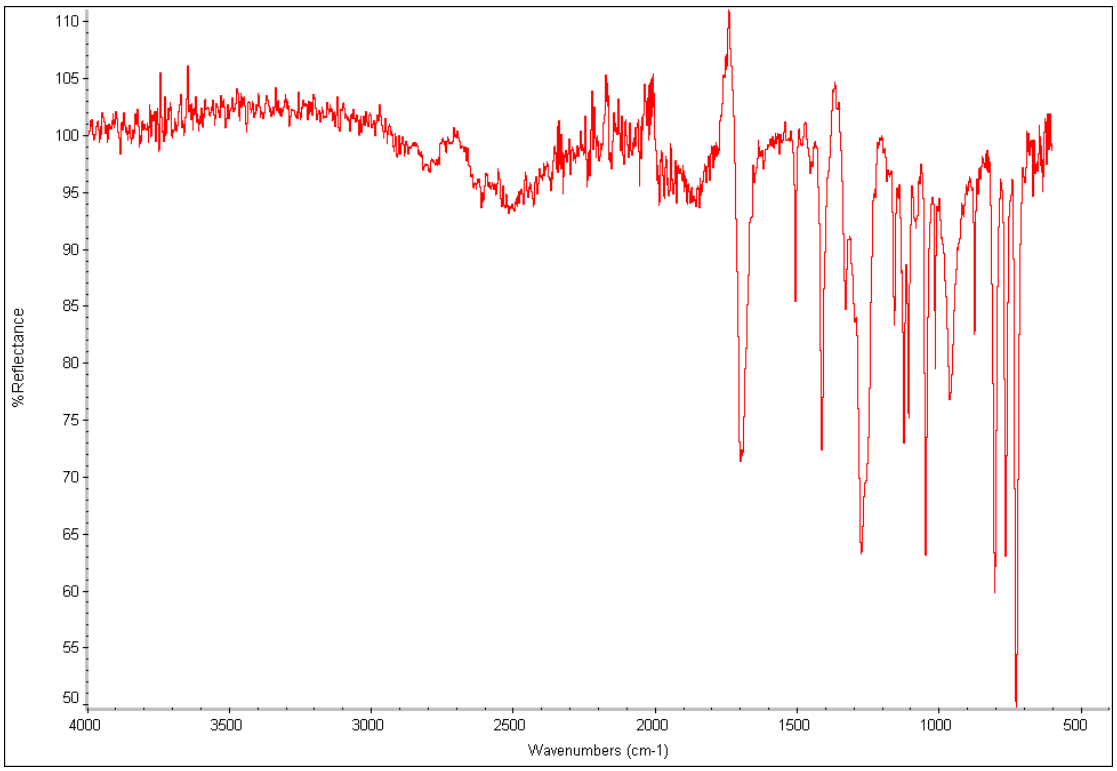

Figure S13. IR spectrum of pyrazine:terephthalic acid cocrystal

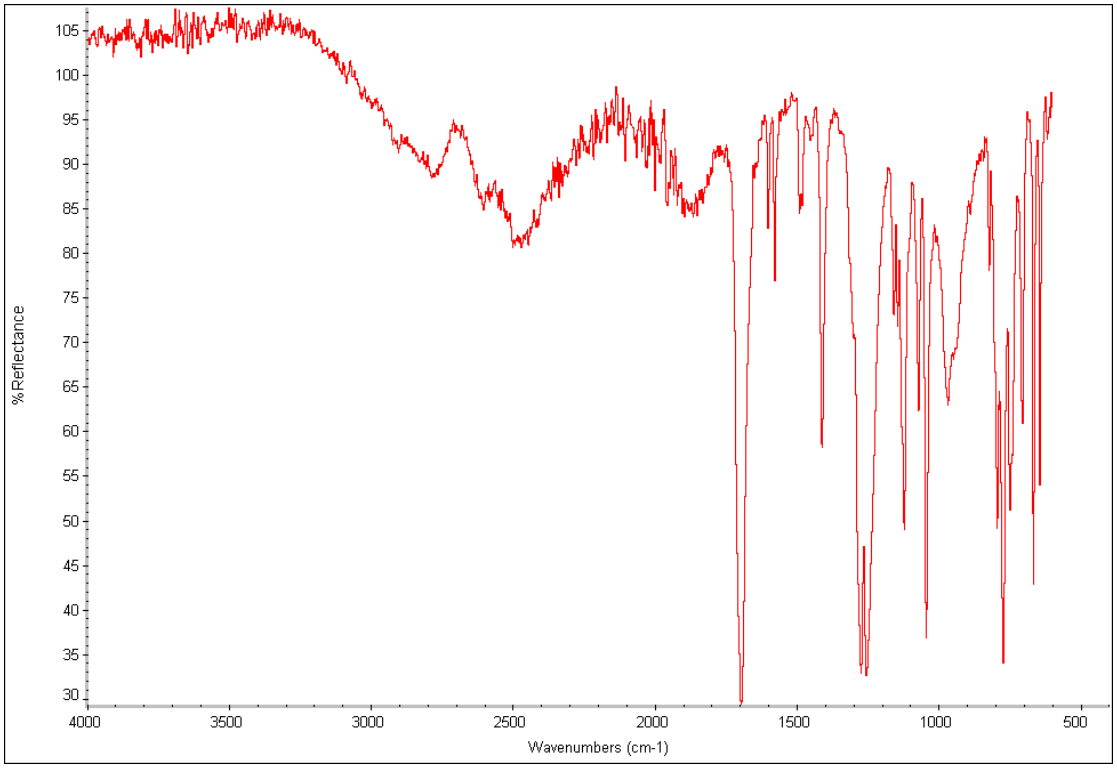

Figure S14. IR spectrum of pyrazine: phthalic acid cocrystal

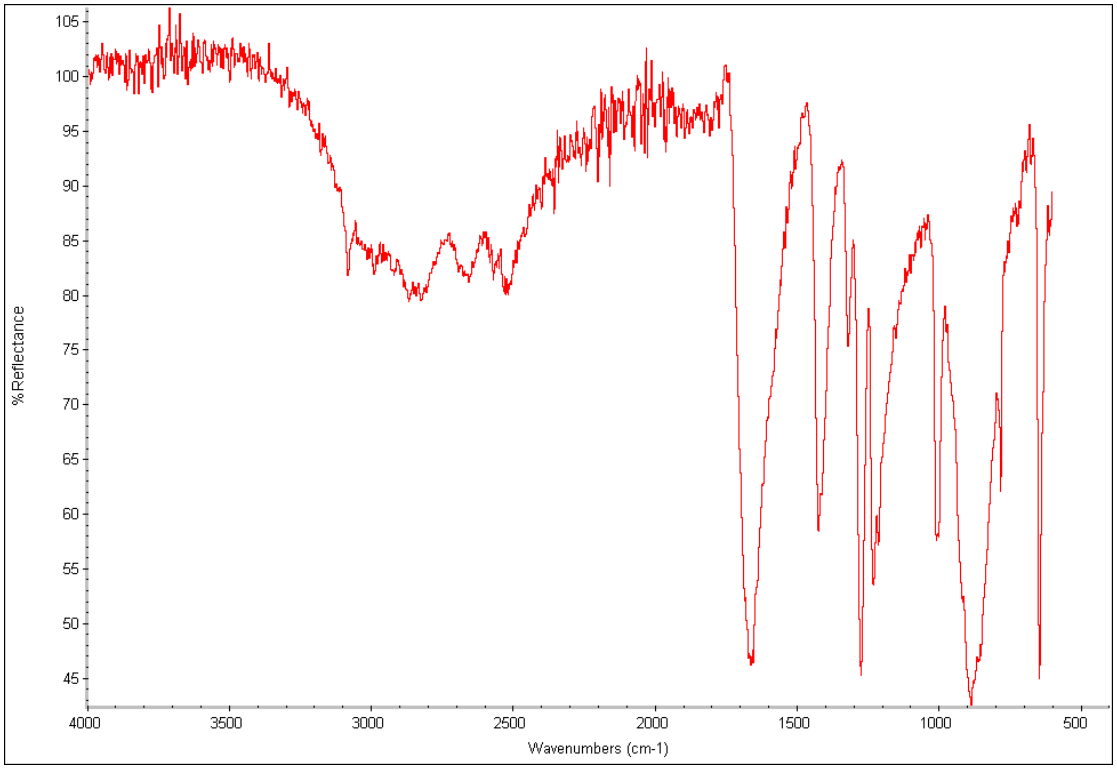

Figure S15. IR spectrum of pyrazine:fumaric acid cocrystal

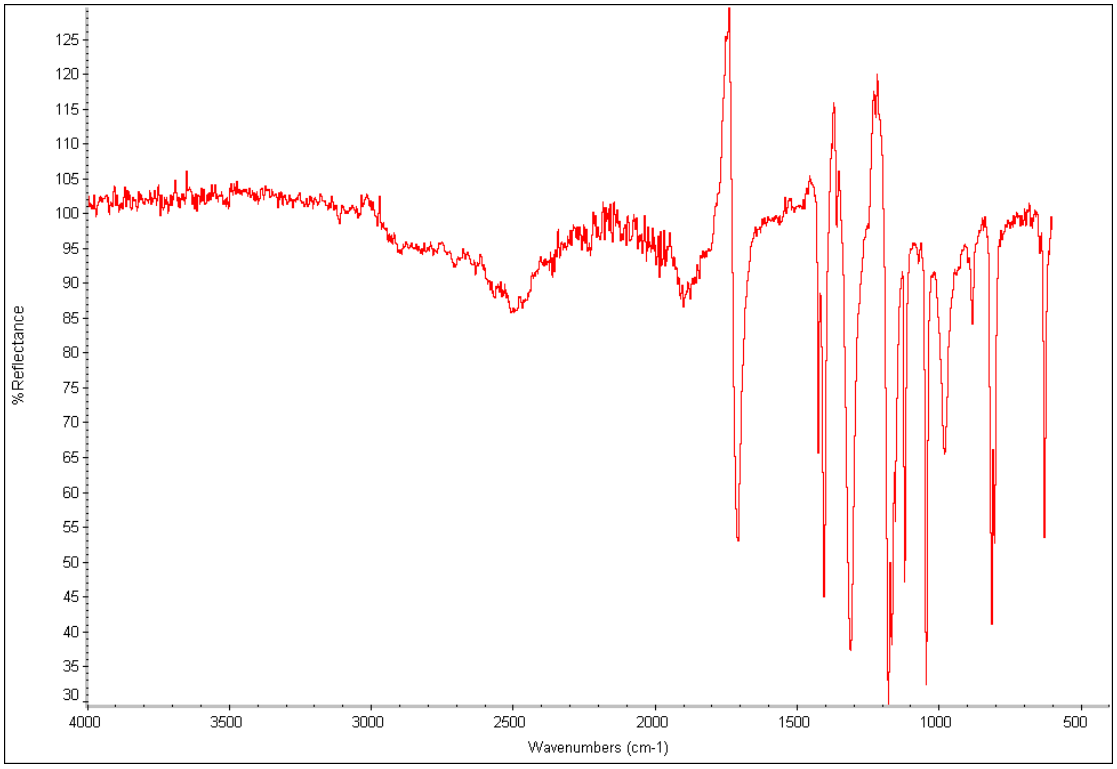

Figure S16. IR spectrum of pyrazine:succinic acid cocrystal

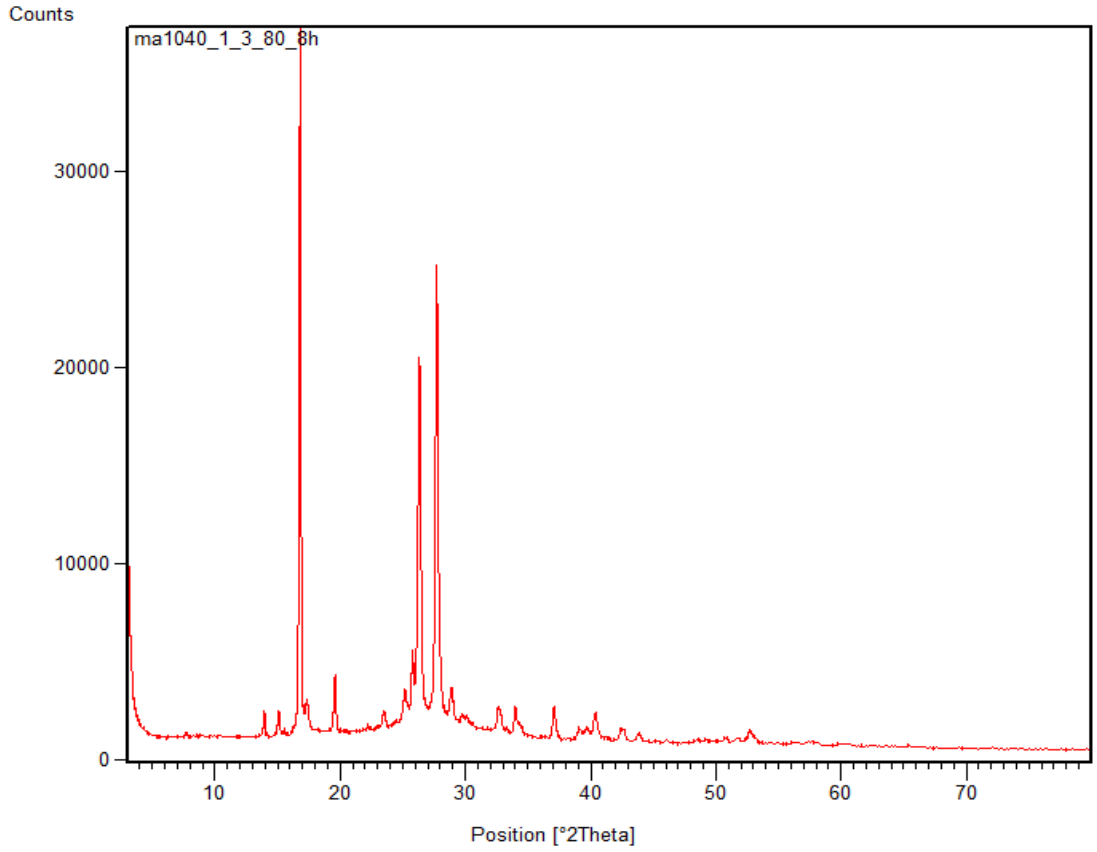

Figure S17. PXRD pattern of pyrazine:terephthalic acid cocrystal

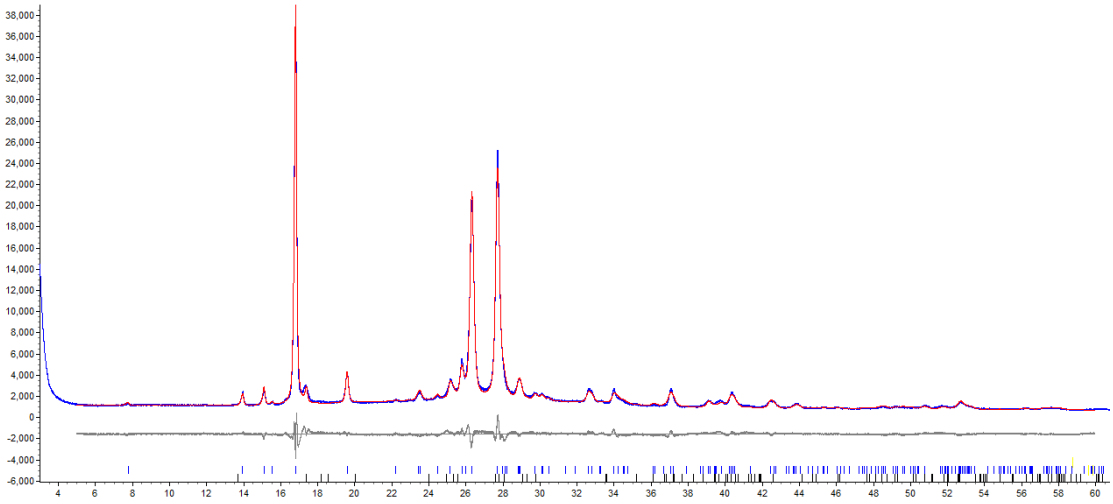

Figure S18. Rietveld refinement of the pyrazine:terephthalic acid cocrystal. The blue outline shows the experimentally observed diffracted pattern, the red curve shows the Rietveld fit and the grey outline marks the difference between the calculated fit and the experimental pattern. Quantitative phase analysis suggests the presence of 3% of terephthalic acid form II (refcode TEPTH12) impurity.

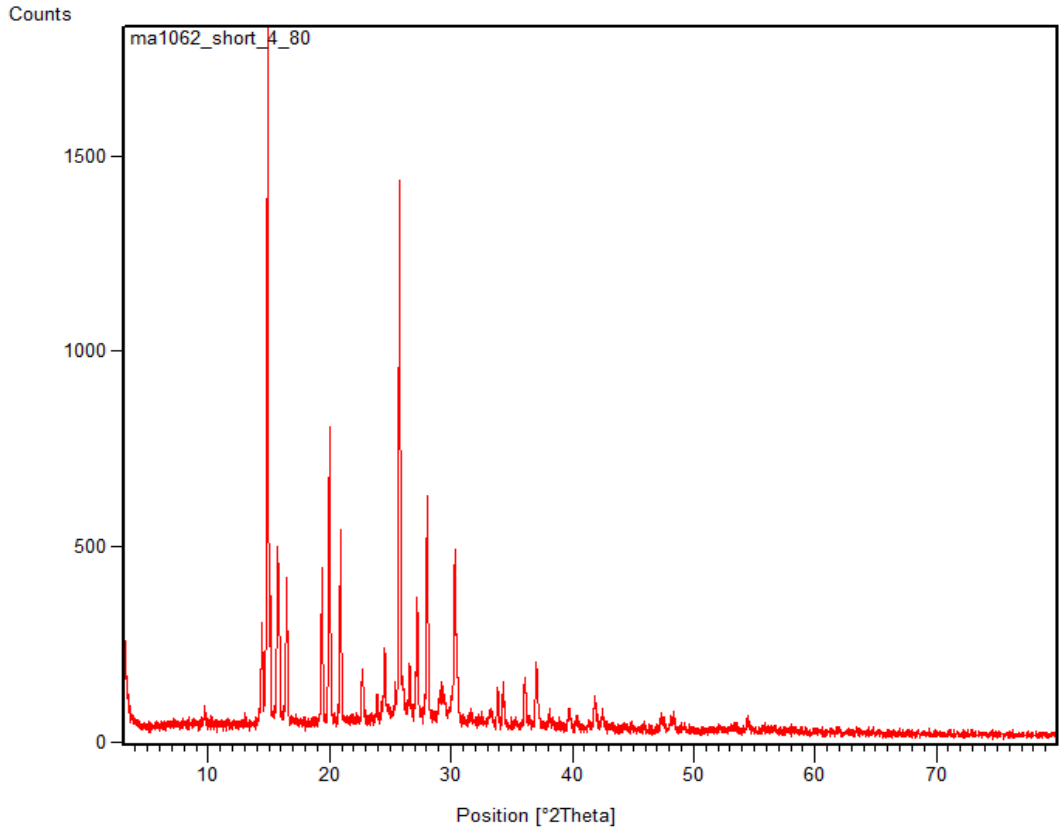

Figure S19. PXRD pattern of pyrazine: phthalic acid cocrystal

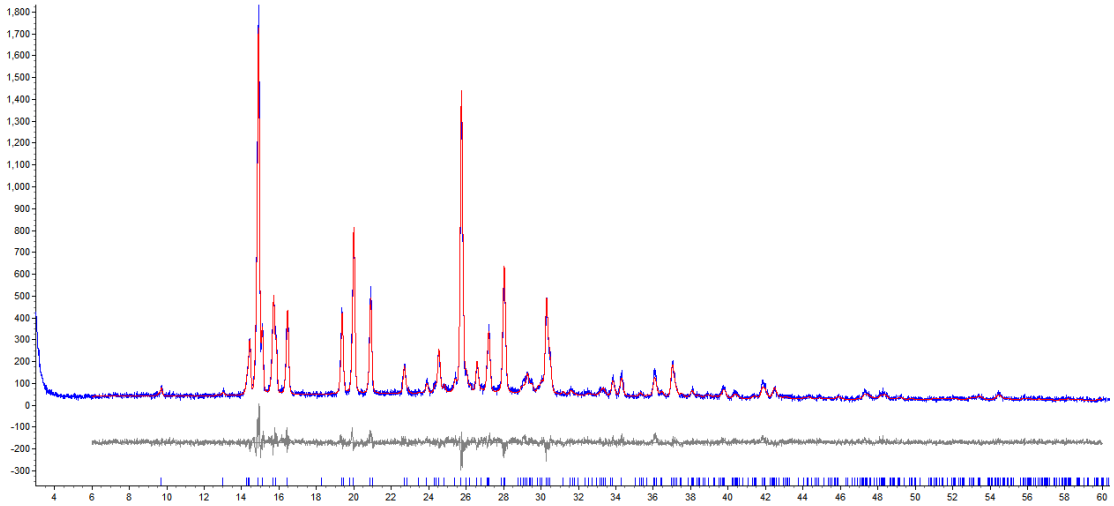

Figure S20. Rietveld refinement of the pyrazine:phthalic acid cocrystal.

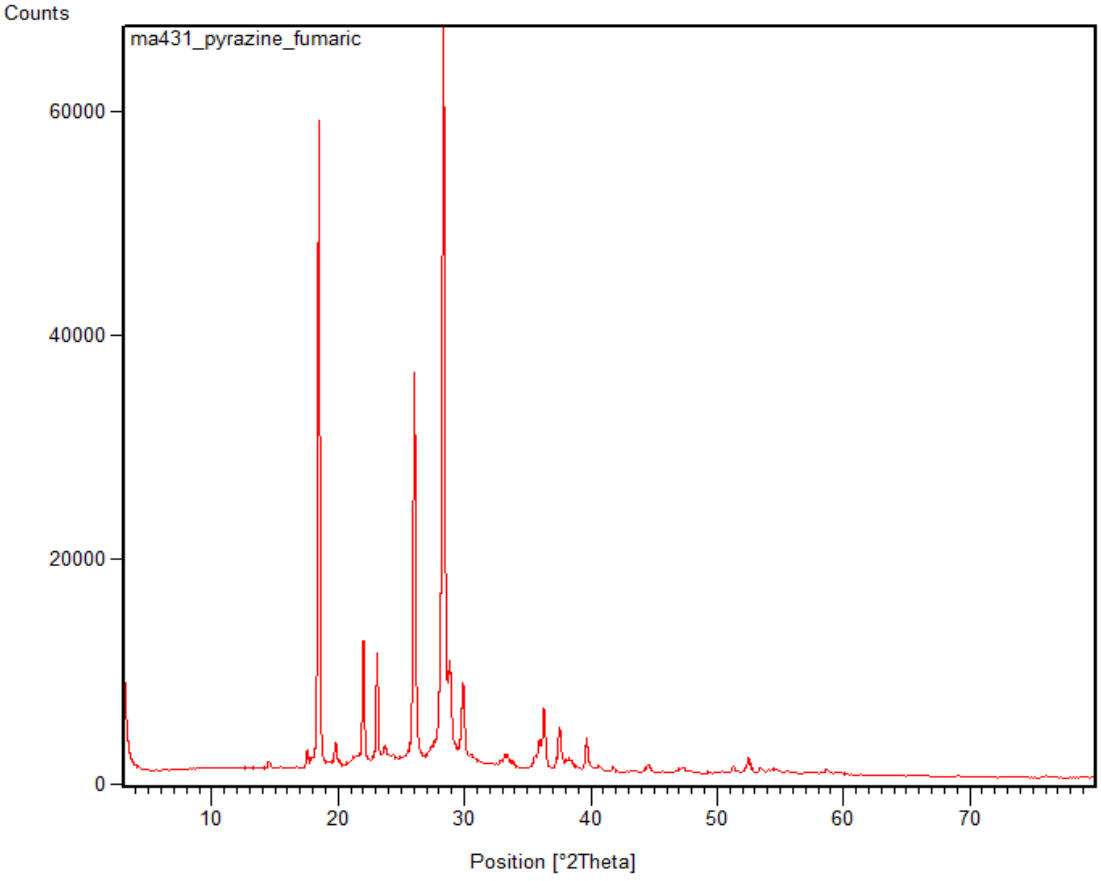

Figure S21. PXRD pattern of pyrazine:fumaric acid cocrystal

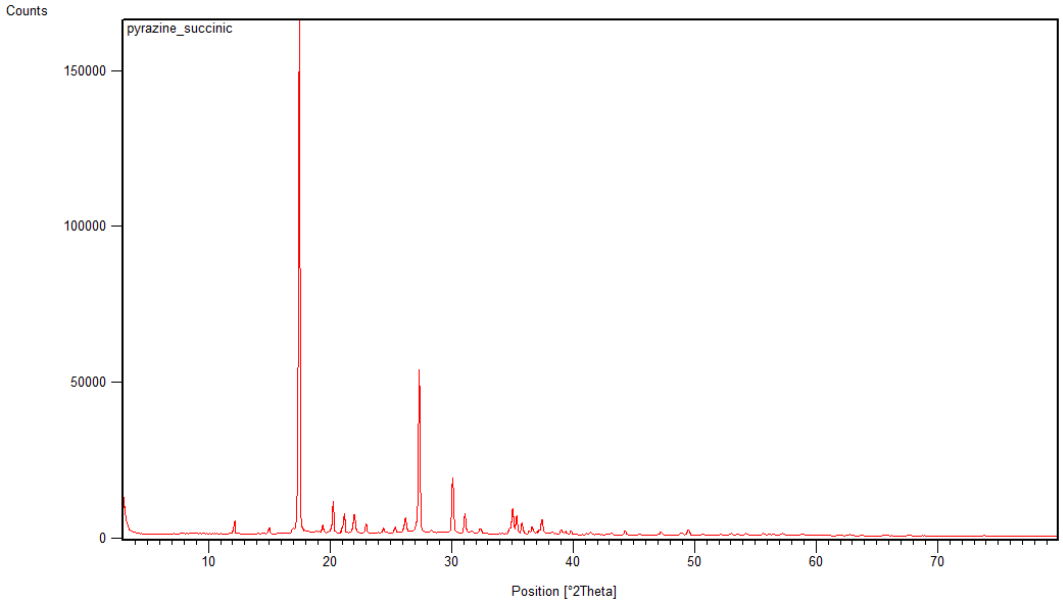

Figure S22. PXRD pattern of pyrazine:succinic acid cocrystal

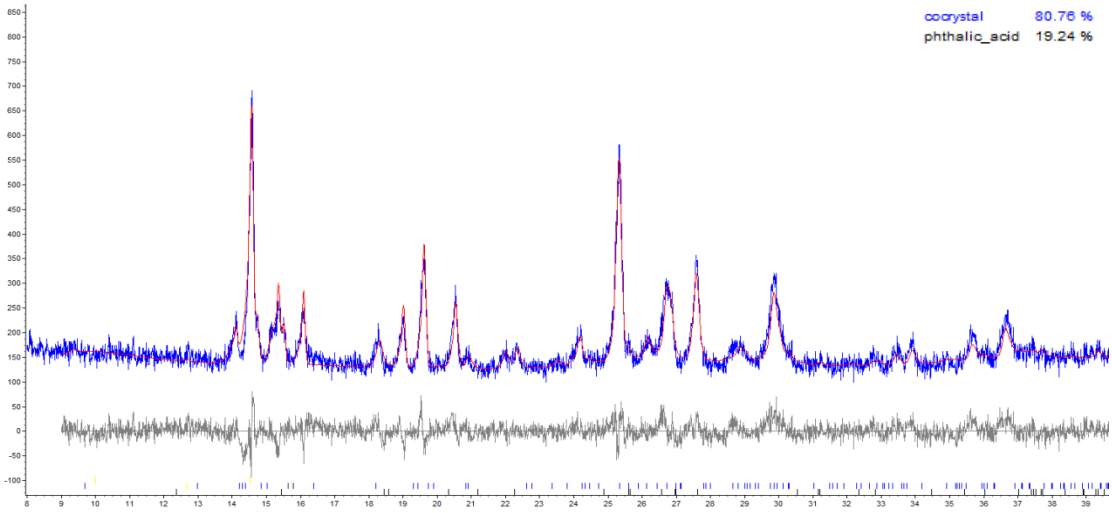

Figure S23. Example of Rietveld refinement of a PXRD pattern recorded on a sample of pyrazine:phthalic acid cocrystal recorded during the kinetics measurement. Refinement of the scale factors of mixture components allows to calculate their corresponding mass fractions (shown in the top right corner).

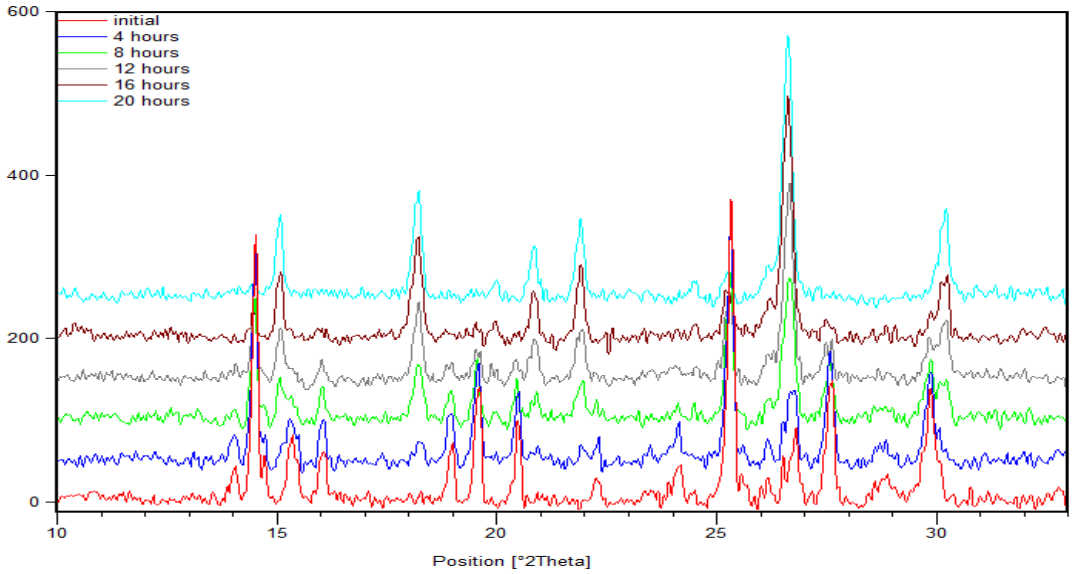

Figure S24. X-ray powder patterns showing the conversion of pyr:pht cocrystal into phthalic acid. The patterns were recorded at 25°C temperature and room humidity. The most prominent peaks corresponding to the cocrystal are at 2θ 14.5°, 19.6°, 25.3° and 29.9°. The major peaks corresponding to phthalic acid are at 2θ 15.1°, 18.2°, 26.6° and 30.2°.

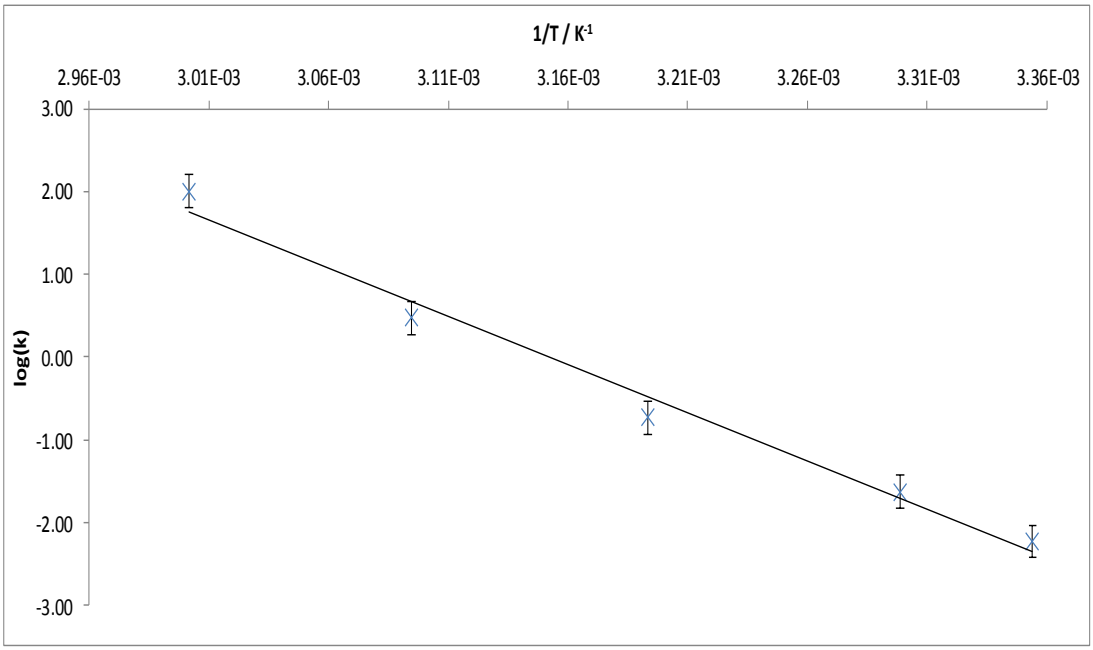

Figure S25. Arrhenius plot describing the dependence of **pyr:pht** cocrystal dissociation rate on temperature