

Supplementary Material

Exploring the relationship between cocrystal stability and symmetry: is Wallach's rule applicable to multi-component solids?

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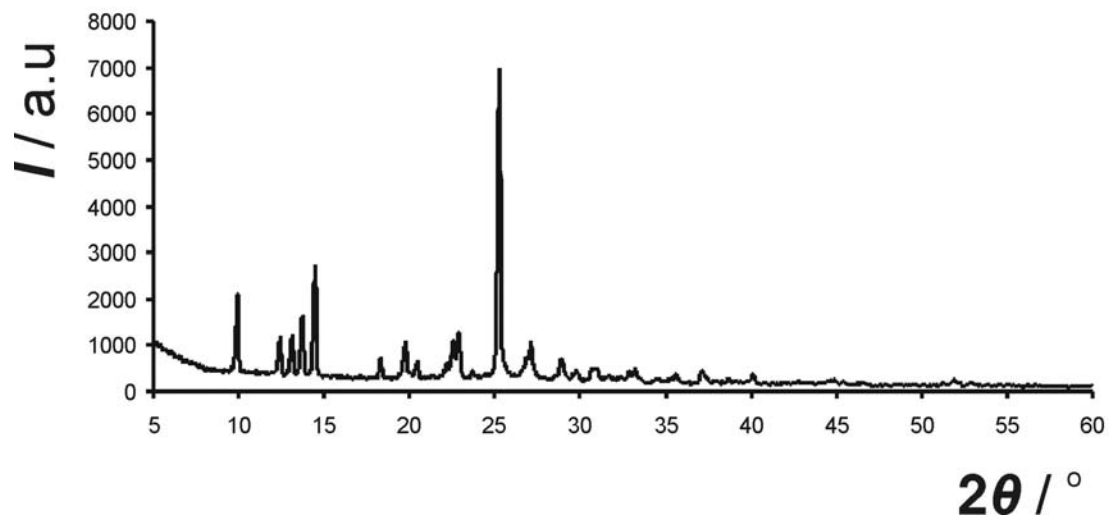


Figure S1. PXRD pattern for the cocrystal of (caf):(D-ma)

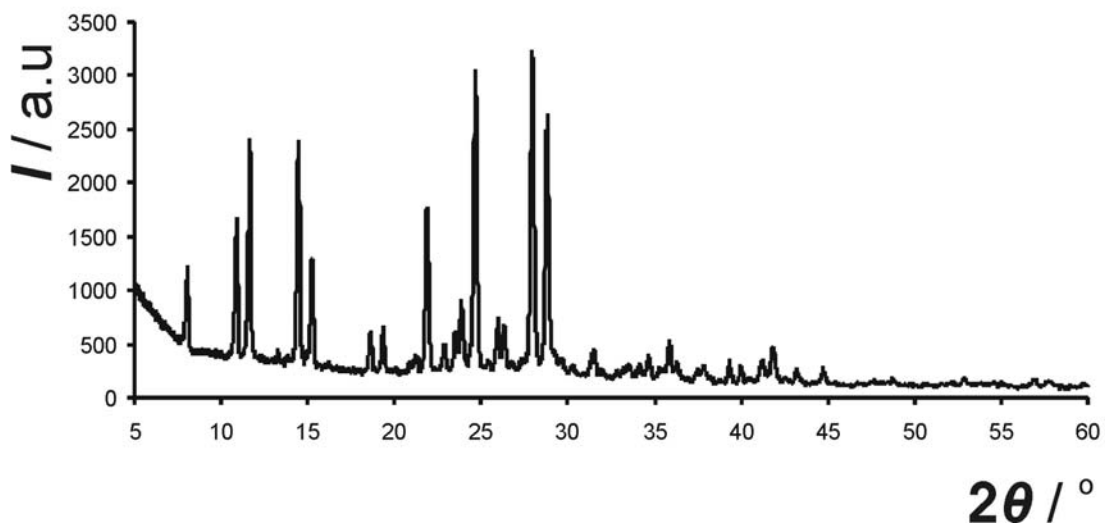


Figure S2. PXRD pattern for the cocrystal of (caf):(DL-ma)

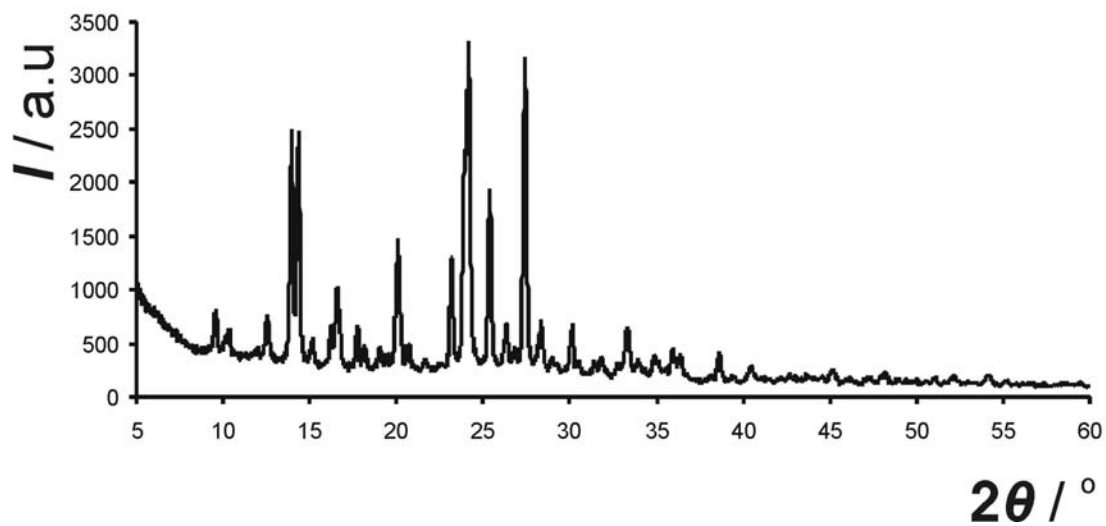


Figure S3. PXRD pattern for the cocrystal of (tp)(D-ta)

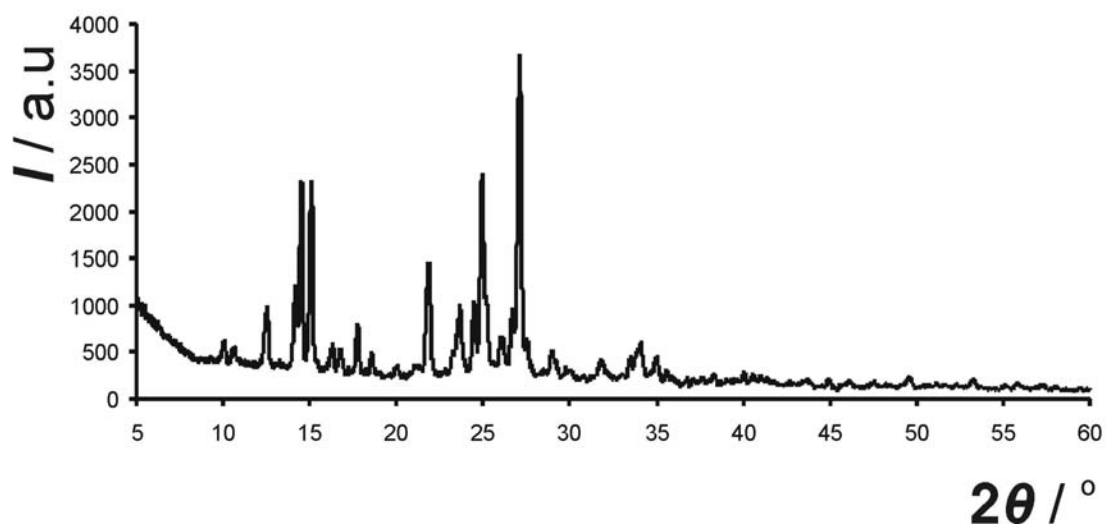


Figure S4. PXRD pattern for the cocrystal of (tp)(DL-ta)

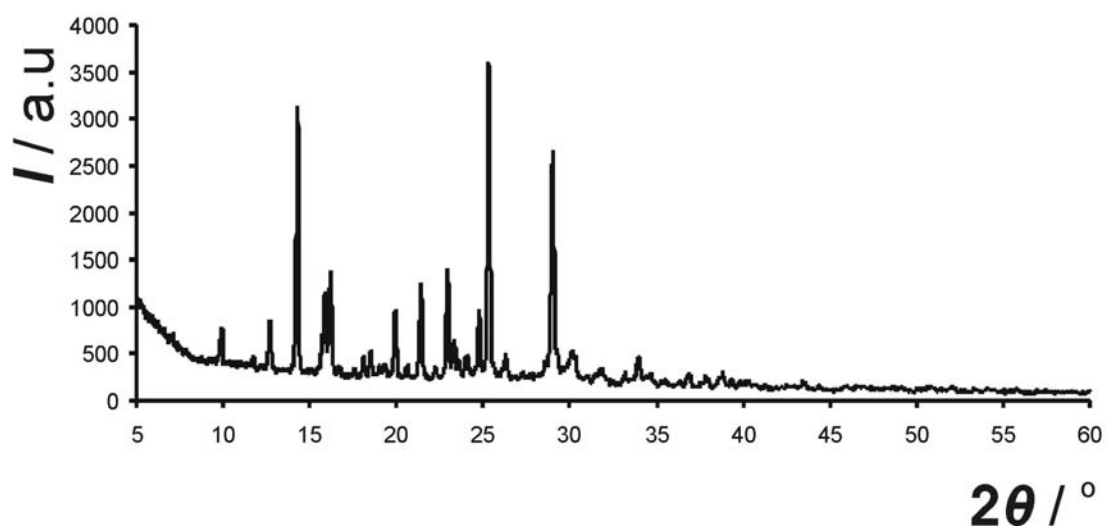


Figure S5. PXRD pattern for the cocrystal of (tp):(D-ma)

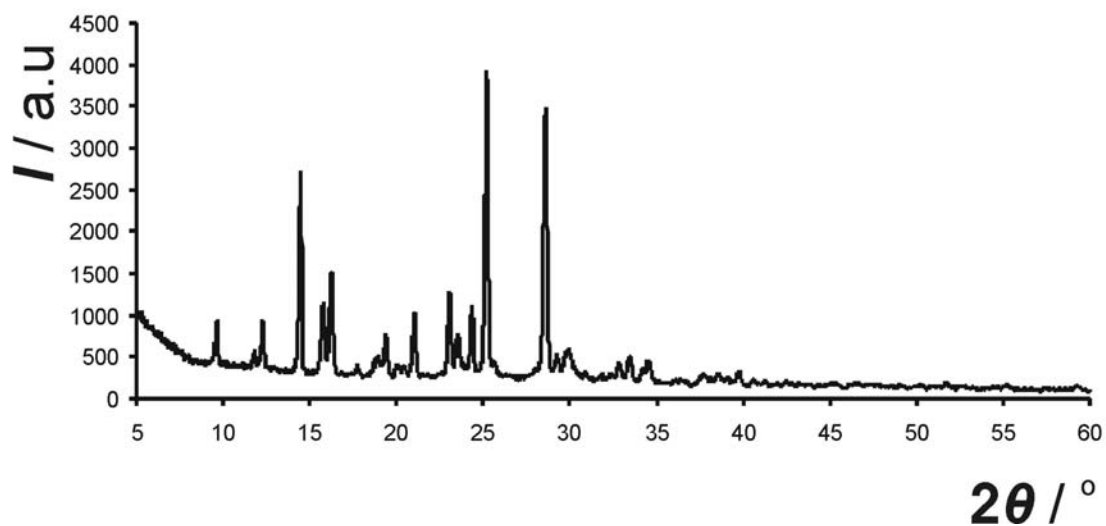


Figure S6. PXRD pattern for the cocrystal of (tp):(DL-ma)

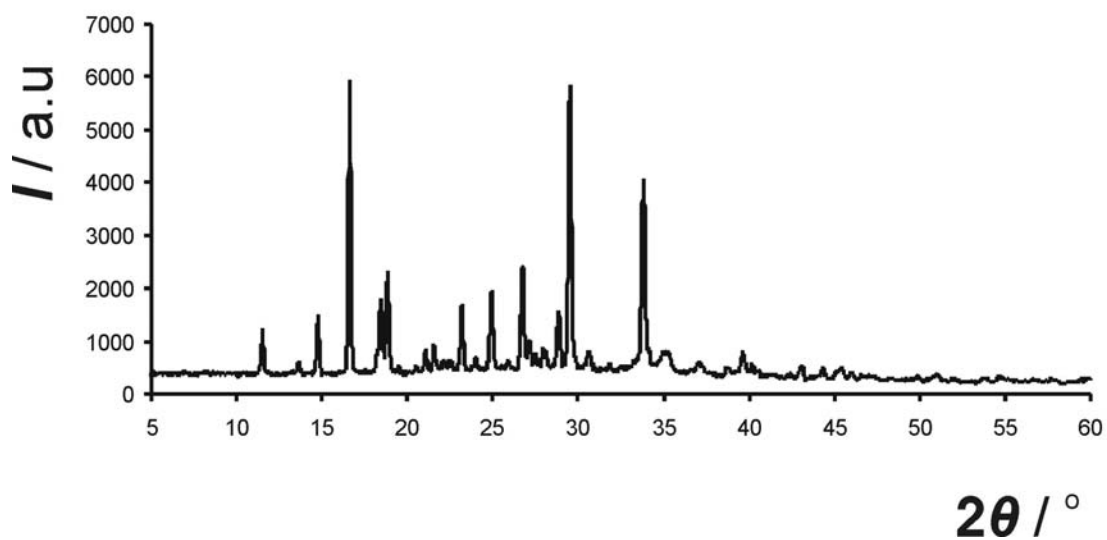


Figure S7. PXRD pattern for the cocrystal of **(tp):(D-ma)** collected using CoK_α radiation.

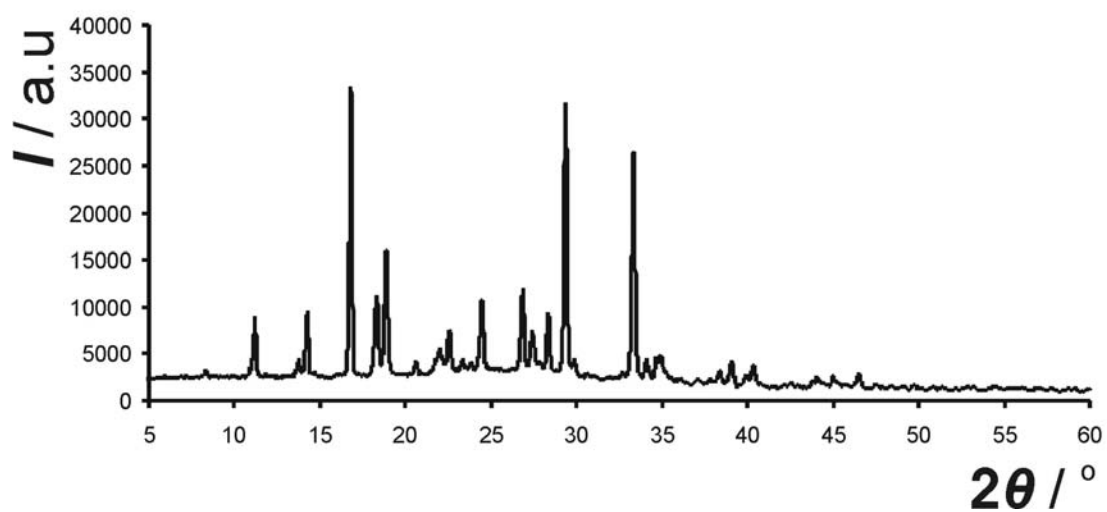


Figure S8. PXRD pattern for the cocrystal of **(tp):(DL-ma)** collected using CoK_α radiation.

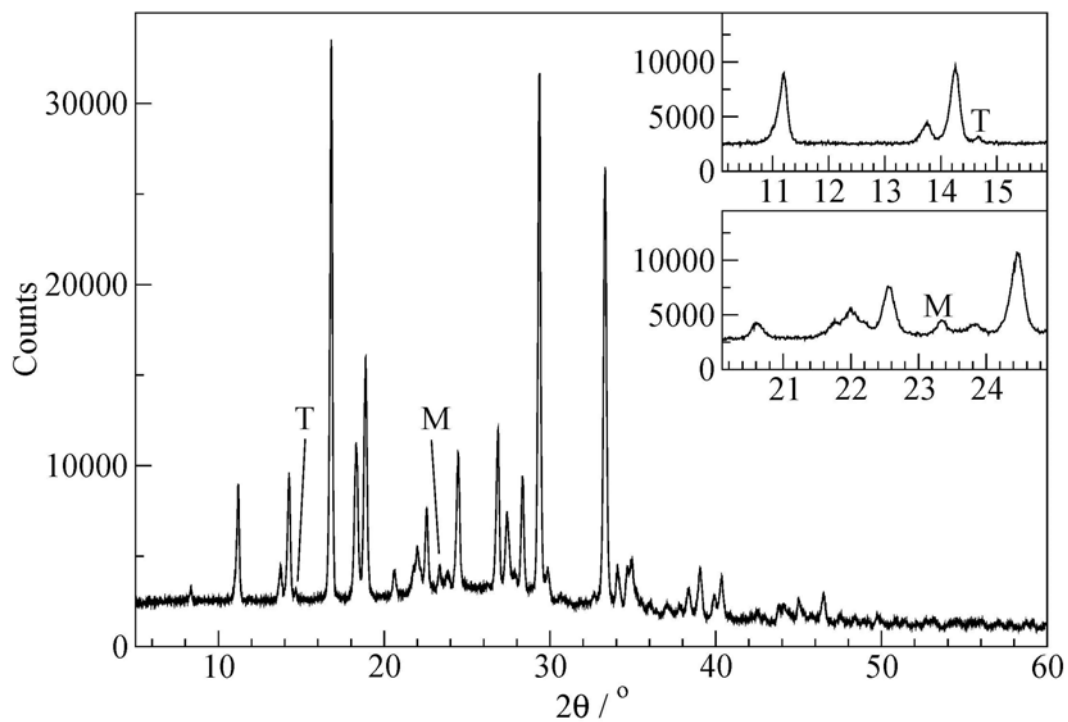


Figure S9. PXR D pattern for the cocrystal of **(tp)(DL-ma)** collected using $\text{CoK}\alpha$ radiation, with marked impurities of theophylline (T, 0.5 %) and DL-malic acid (M, 6.5 %).

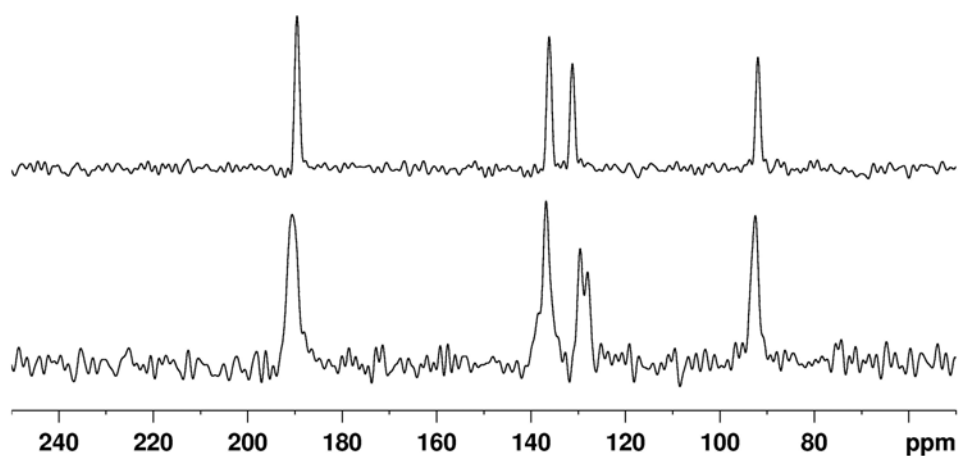


Figure S10. ^{15}N CP-MAS spectra for the cocrystals **(caf)(D-ma)** (bottom) and **(caf)(DL-ma)** (top)

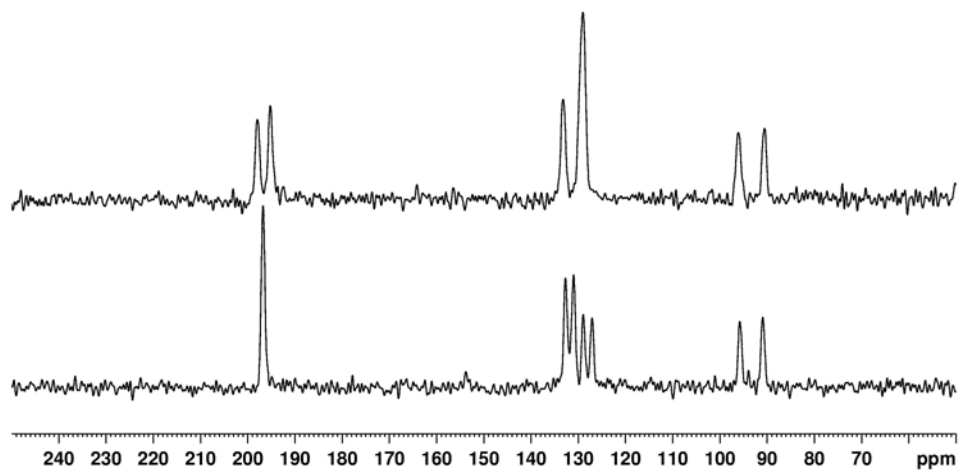


Figure S11. ^{15}N CP-MAS spectra for the cocrystals (tp)(D-ta) (bottom) and (tp)(DL-ta) (top).

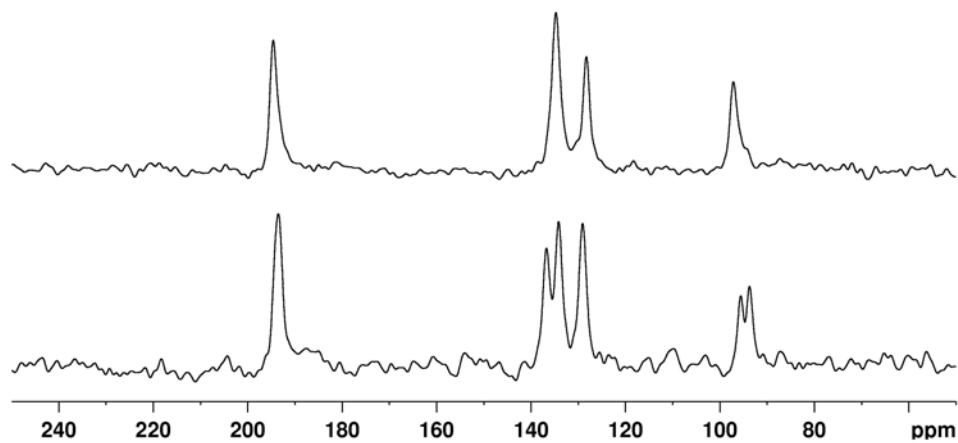


Figure S12. ^{15}N CP-MAS spectra for the cocrystals (tp)(D-ma) (bottom) and (tp)(DL-ma) (top).

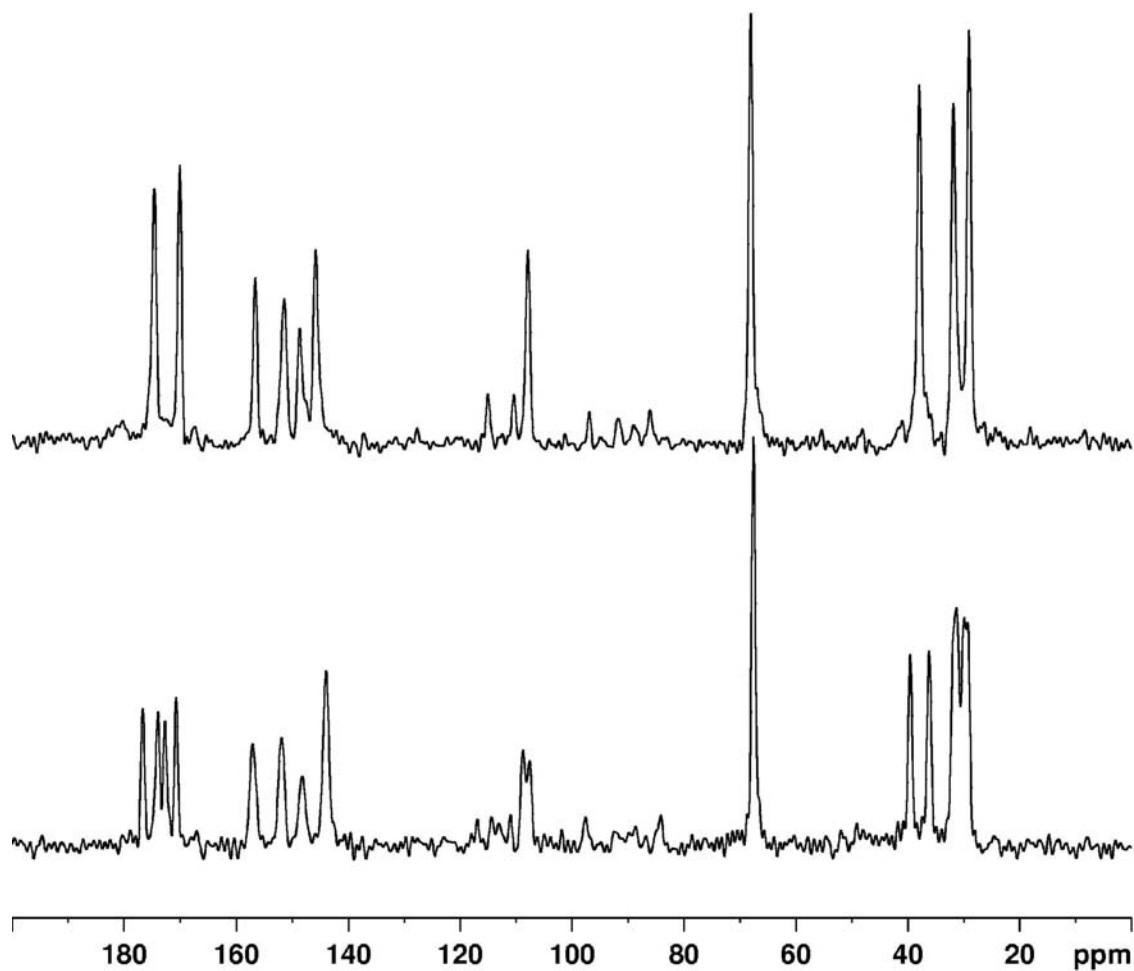


Figure S13. ^{13}C CP-MAS spectra for the cocrystals (**tp**):(D-ma) (bottom) and (**tp**):(DL-ma) (top).

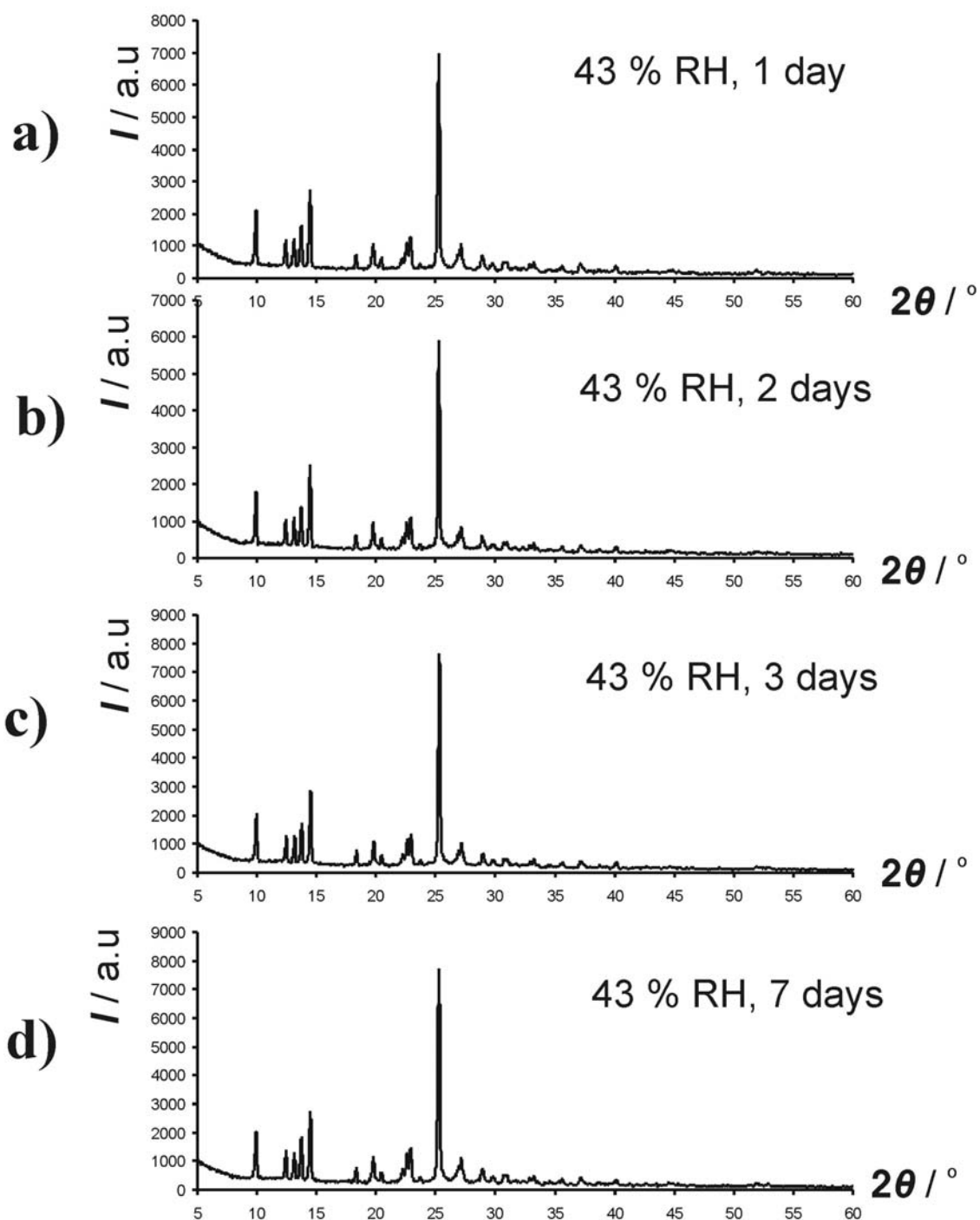


Figure S14. PXRD patterns for the cocrystal of (caf)(D-ma) after exposure to 43% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

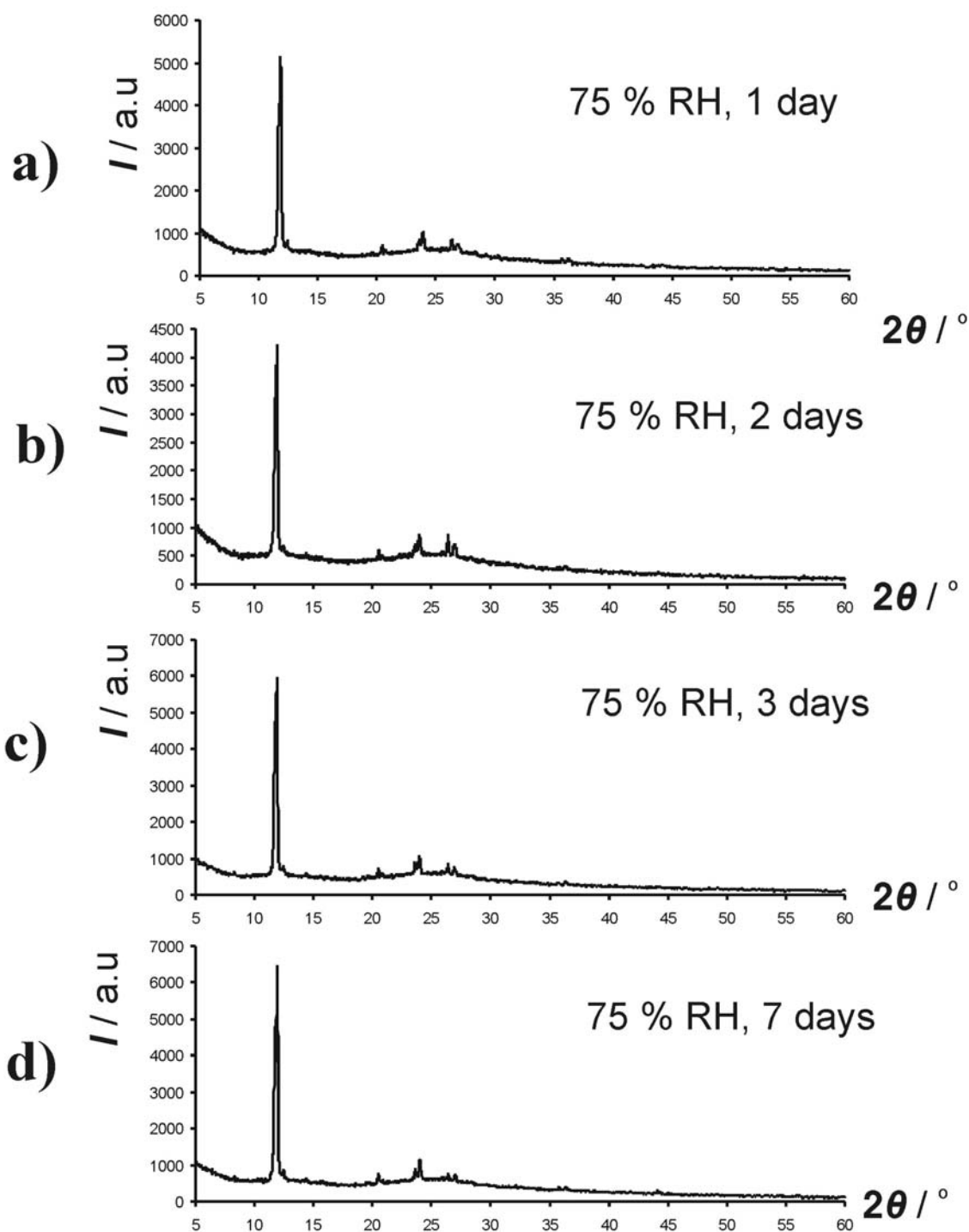


Figure S15. PXRD patterns for the cocrystal of (caf)(D-ma) after exposure to 75% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

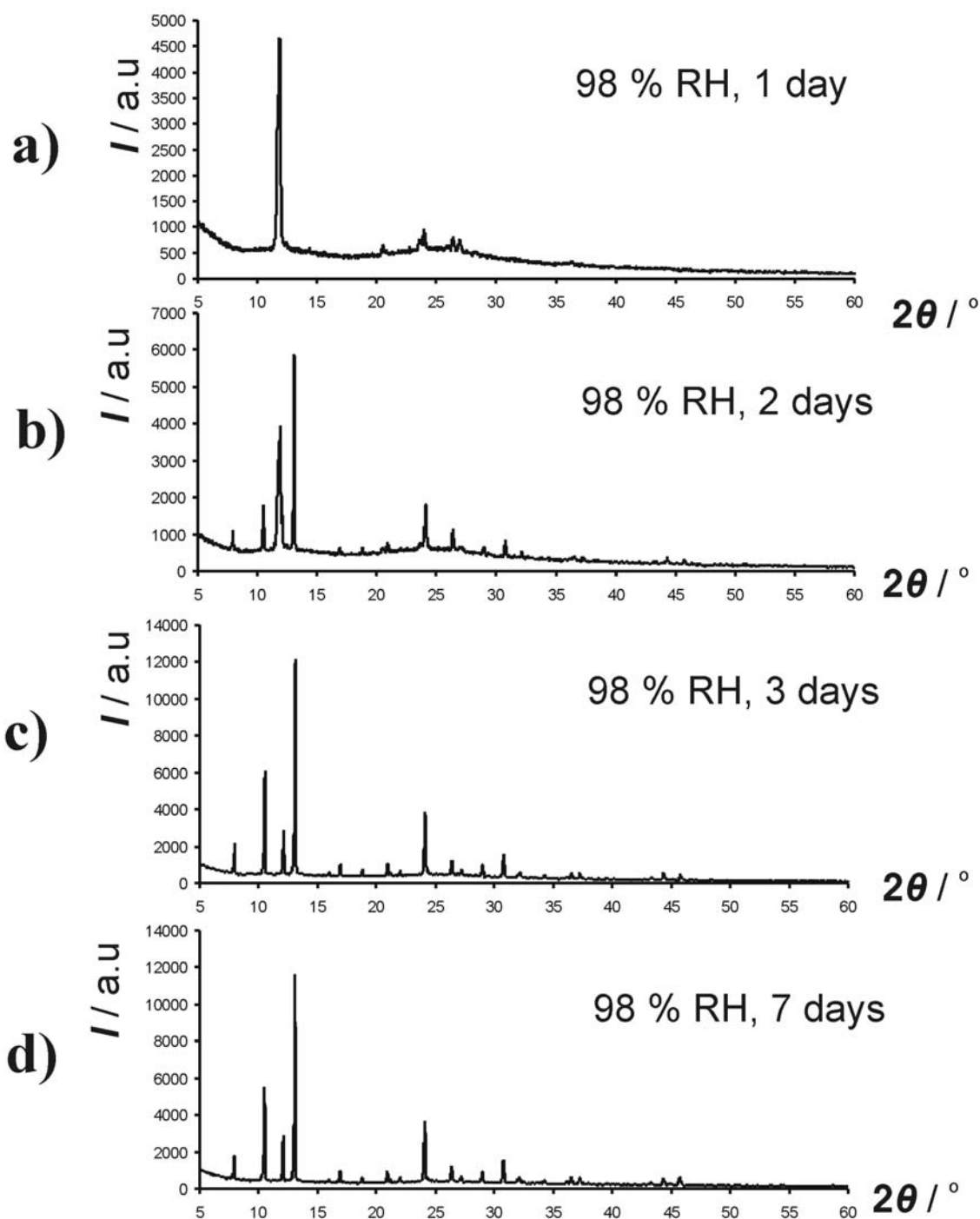


Figure S16. PXRD patterns for the cocrystal of (caf)(D-ma) after exposure to 98% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

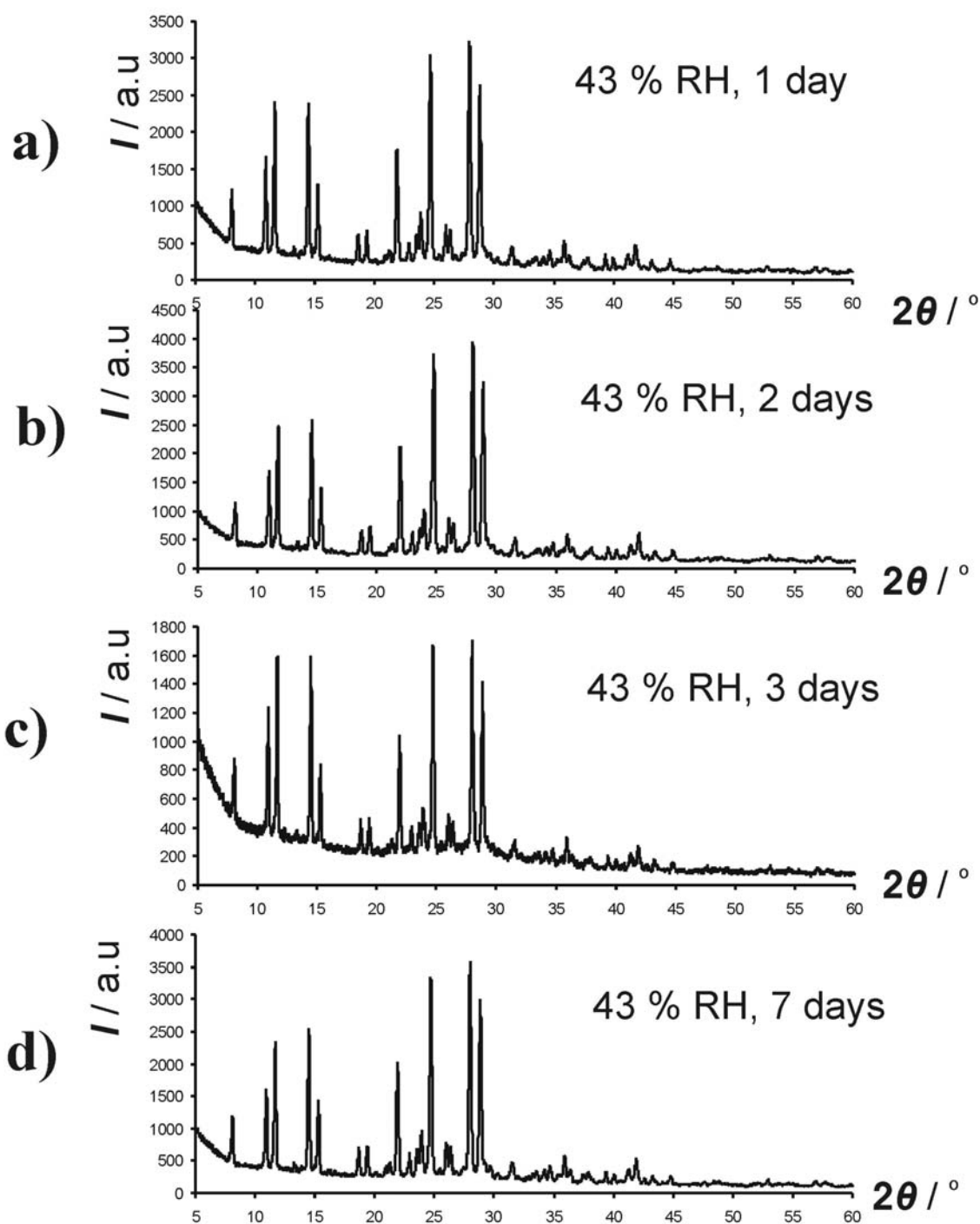


Figure S17. PXRD patterns for the cocrystal of (caf)(DL-ma) after exposure to 43% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

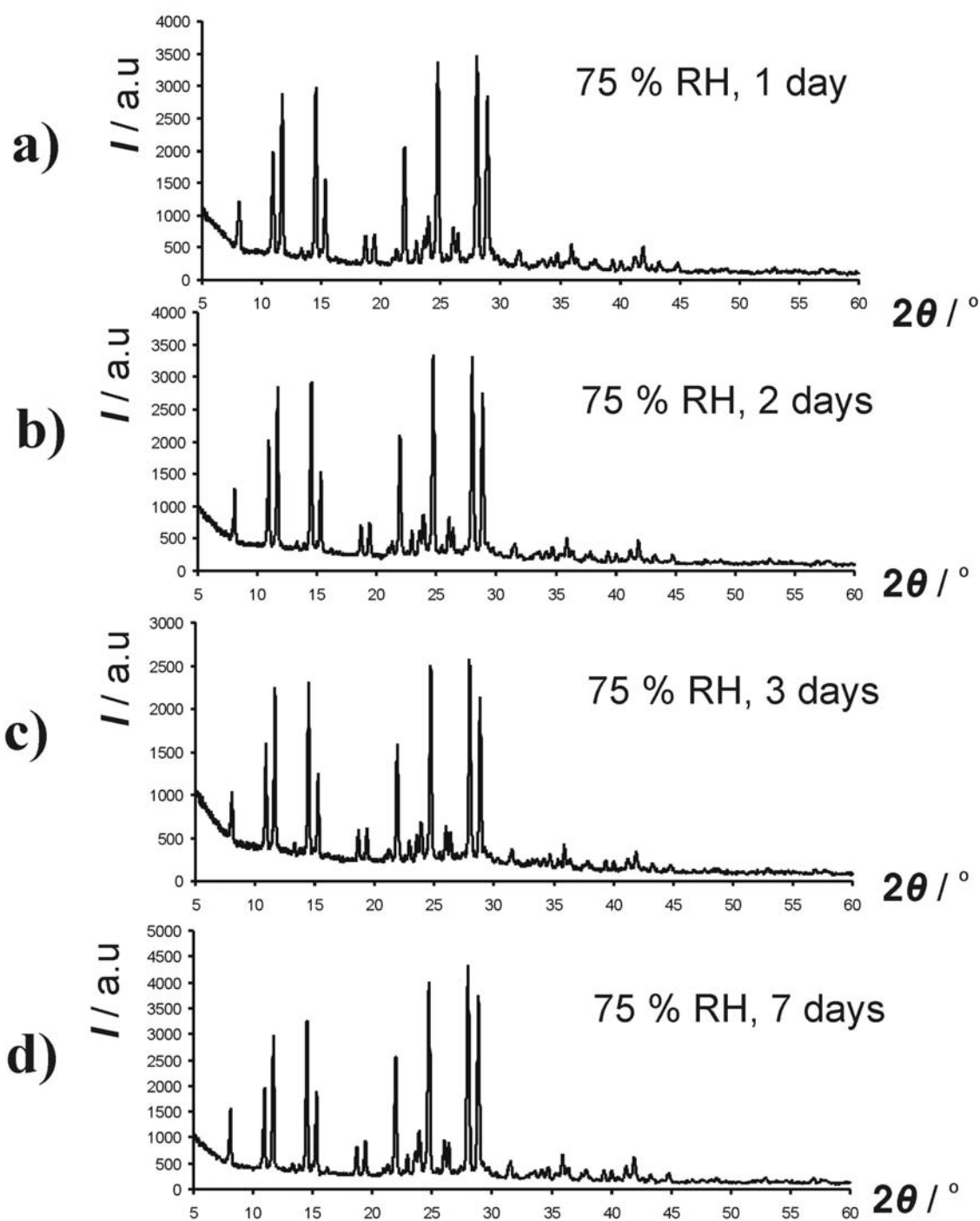


Figure S18. PXRD patterns for the cocrystal of (caf)(DL-ma) after exposure to 75% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

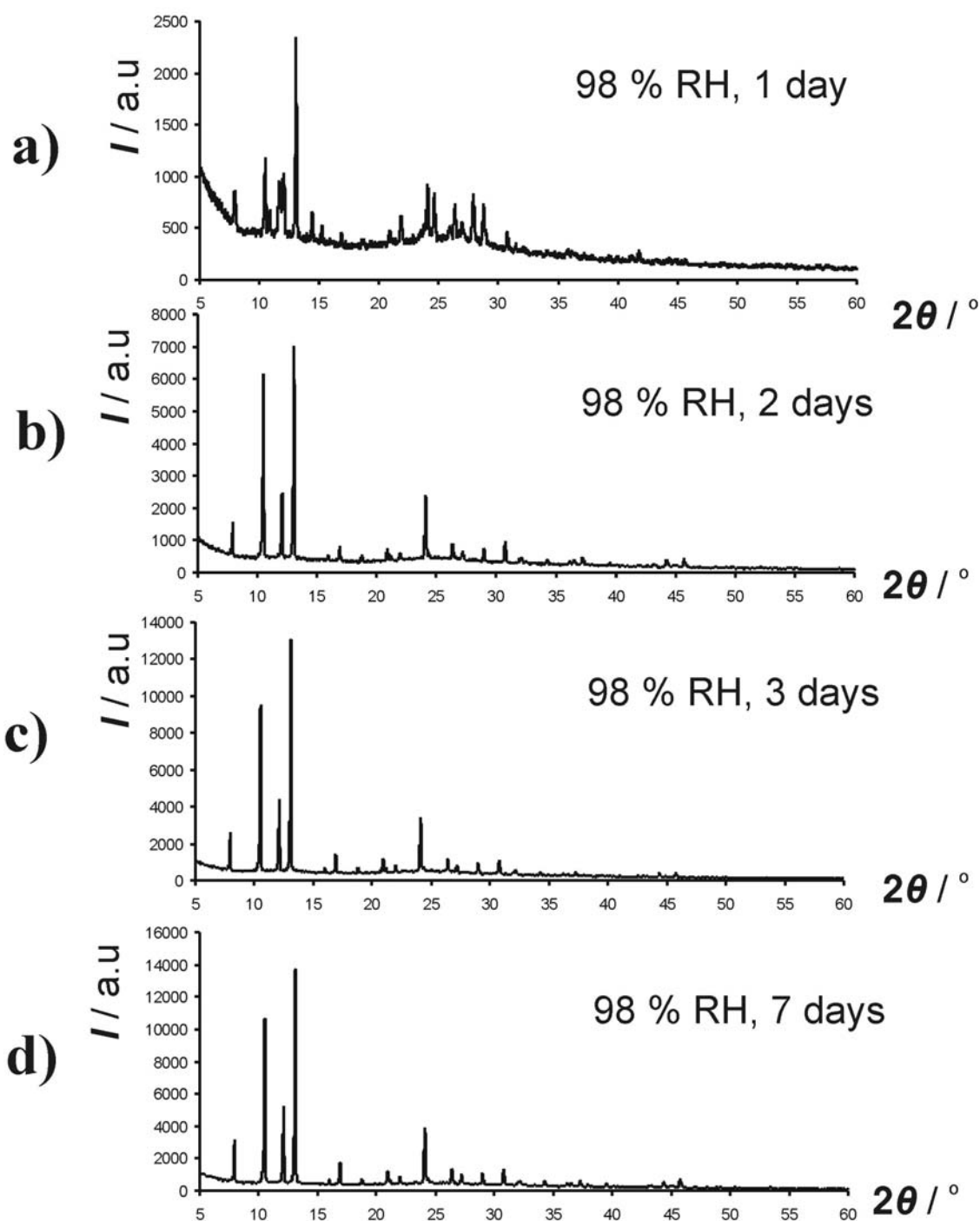


Figure S19. PXRD patterns for the cocrystal of (caf)(DL-ma) after exposure to 98% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

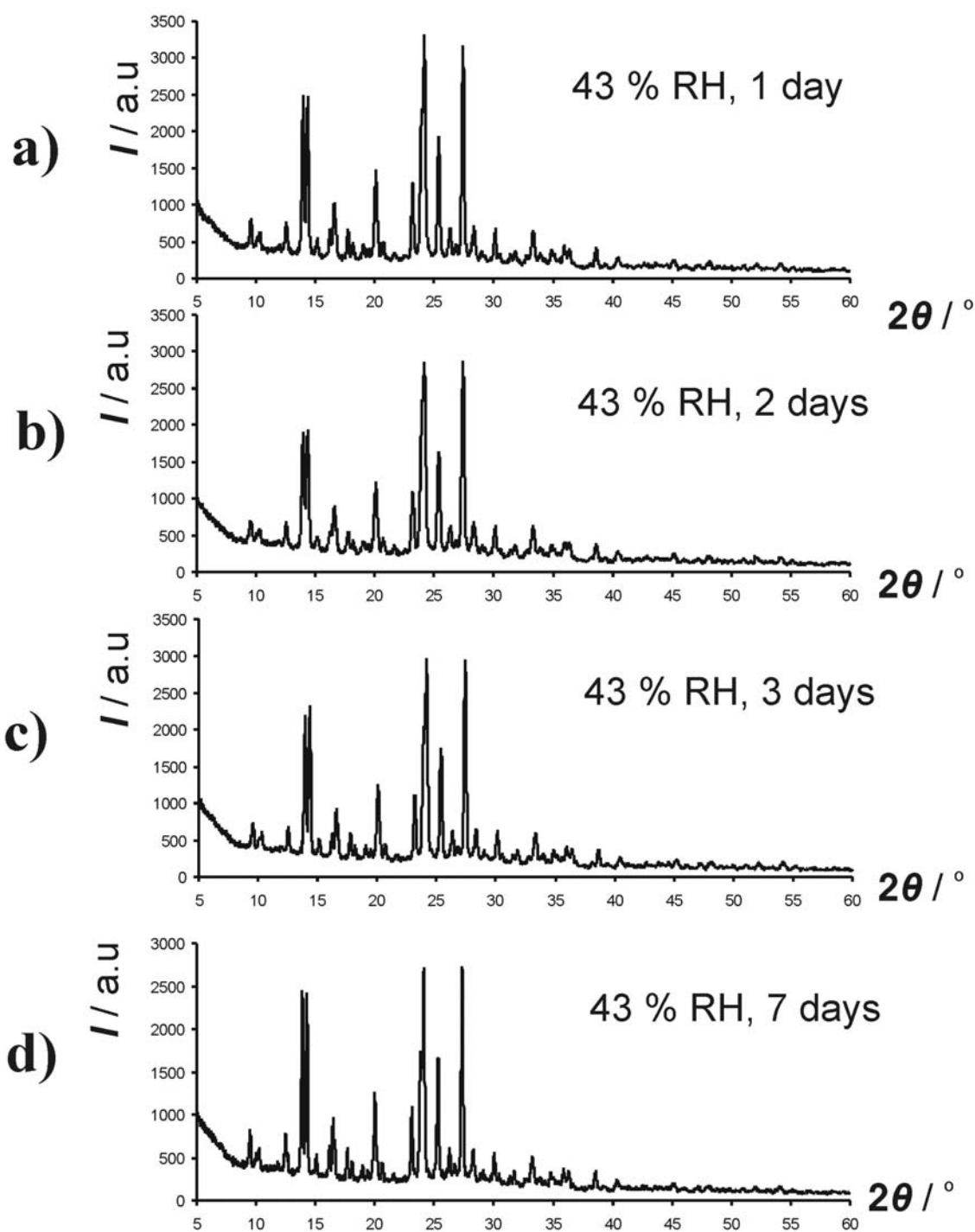


Figure S20. PXRD patterns for the cocrystal of $(tp)_2(D-ta)$ after exposure to 43% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

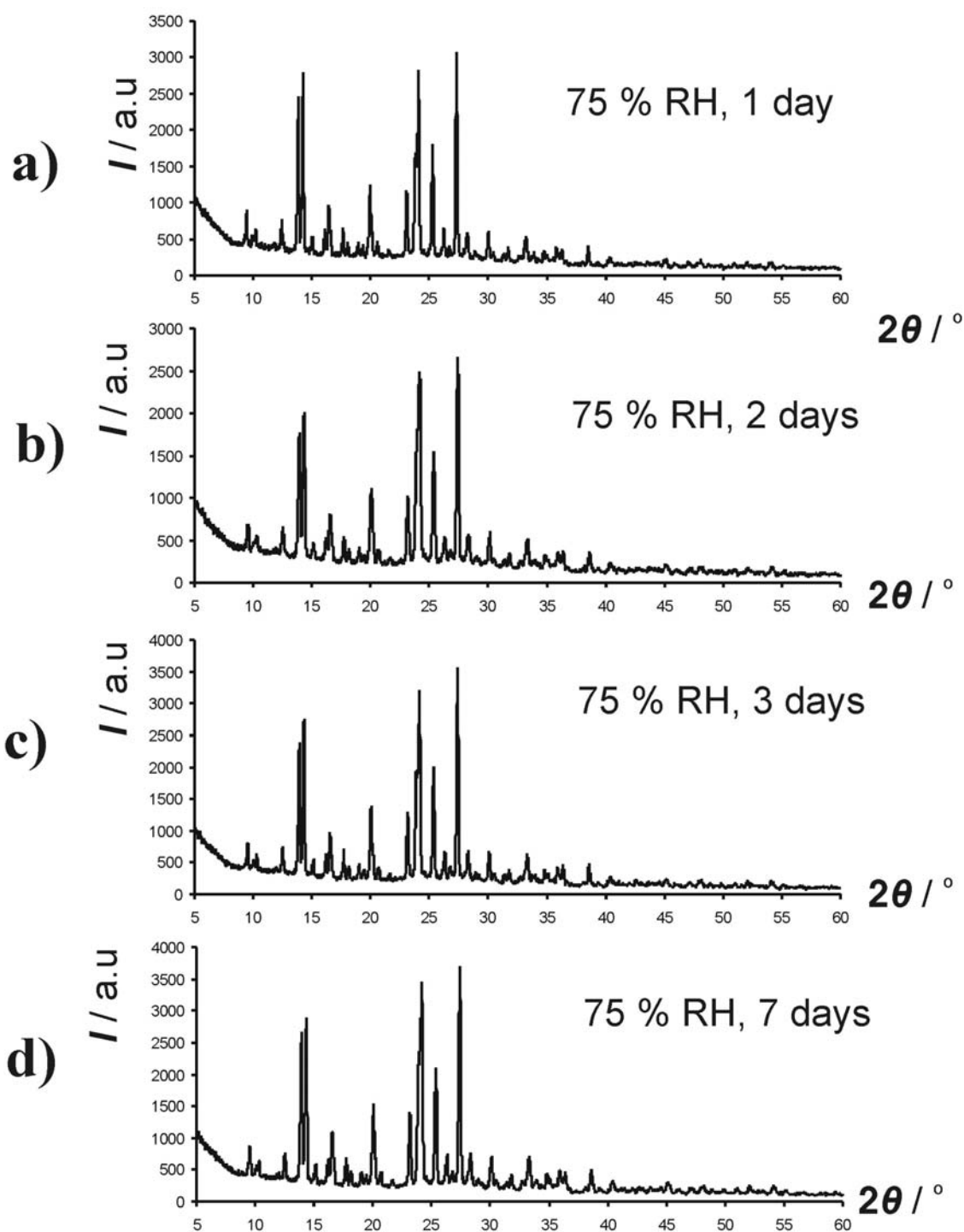


Figure S21. PXRD patterns for the cocrystal of $(\text{tp})_2(\text{D-ta})$ after exposure to 75% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

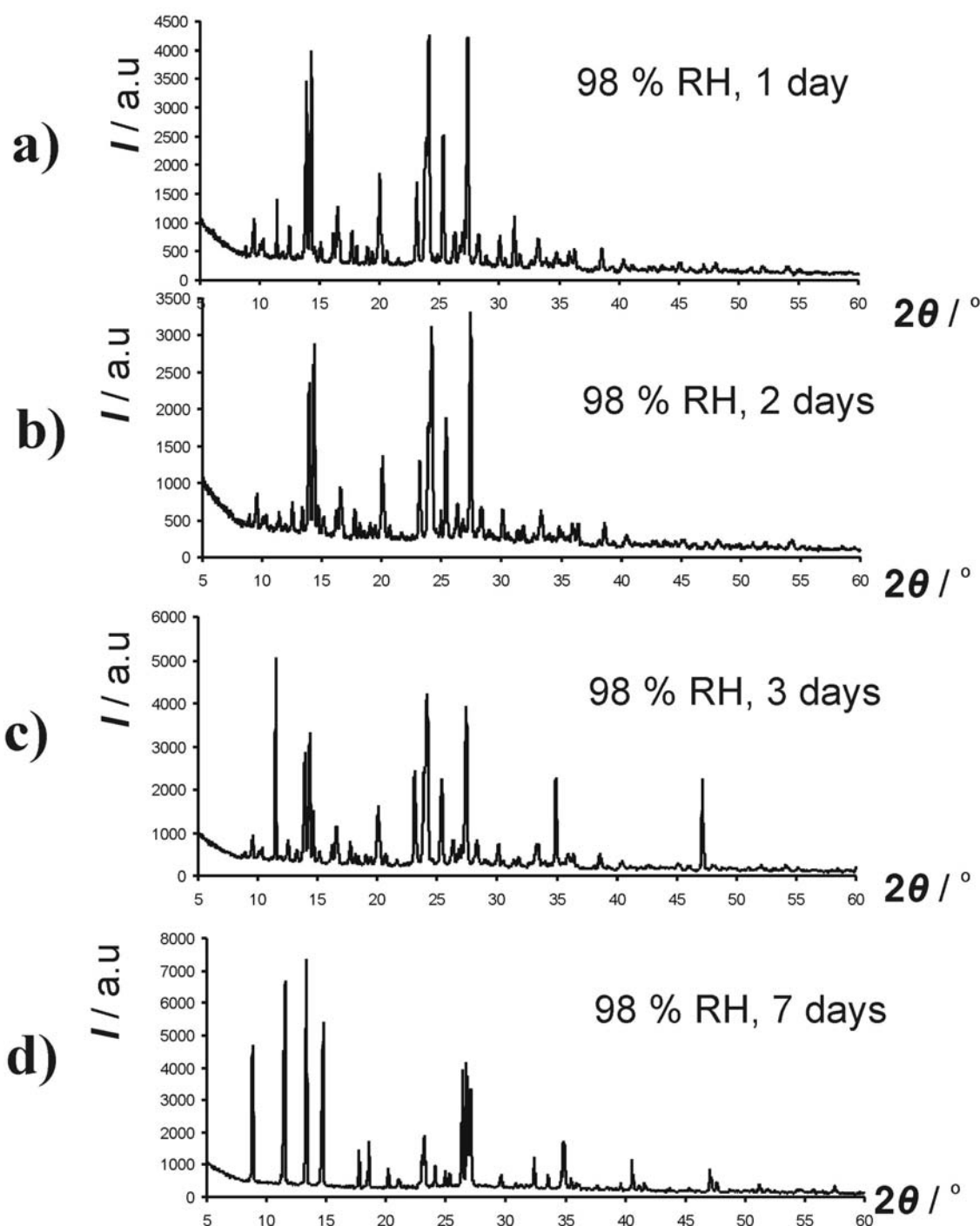


Figure S22. PXRD patterns for the cocrystal of $(\text{tp})_2(\text{D-ta})$ after exposure to 98% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

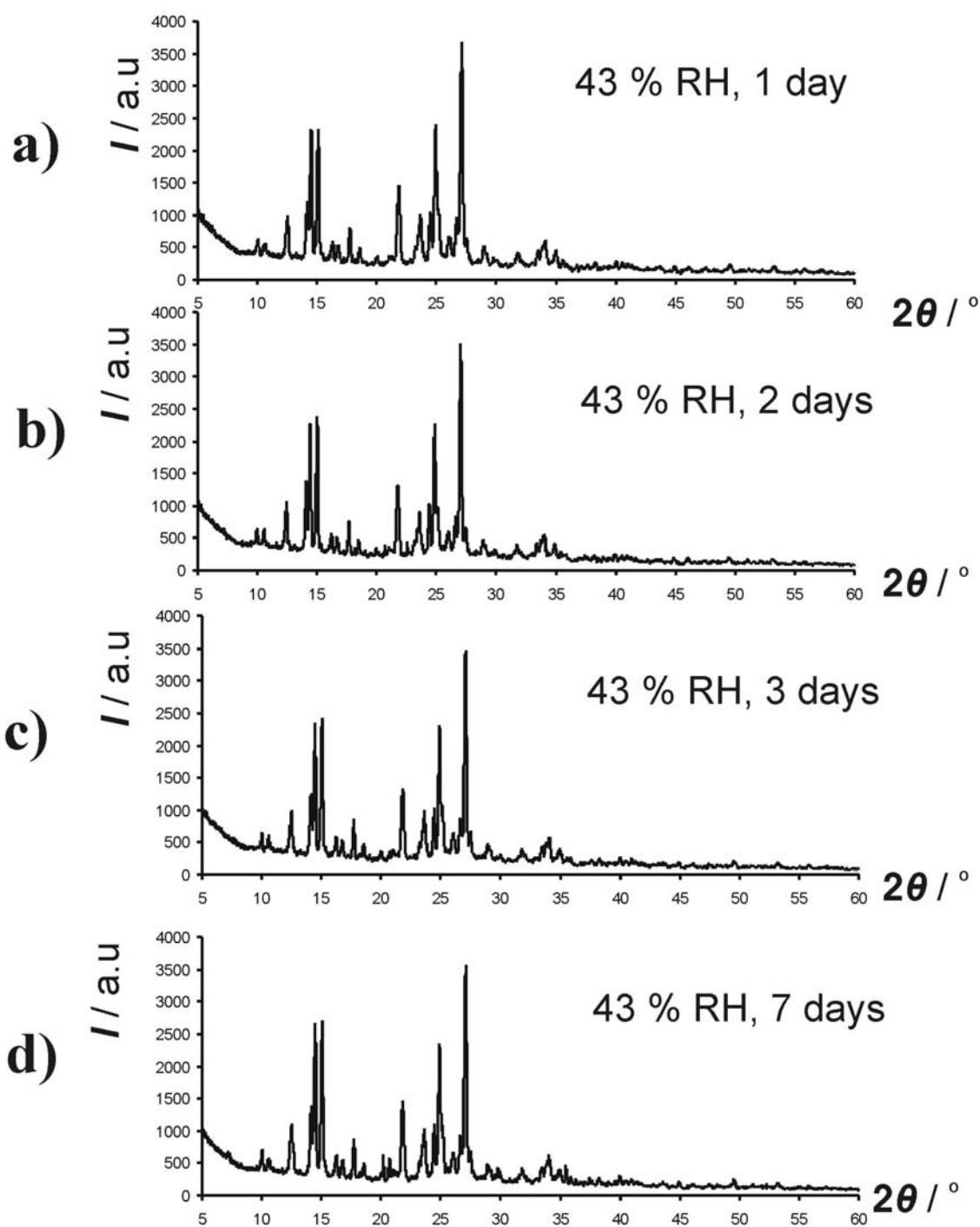


Figure S23. PXRD patterns for the cocrystal of $(tp)_2(DL-ta)$ after exposure to 43% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

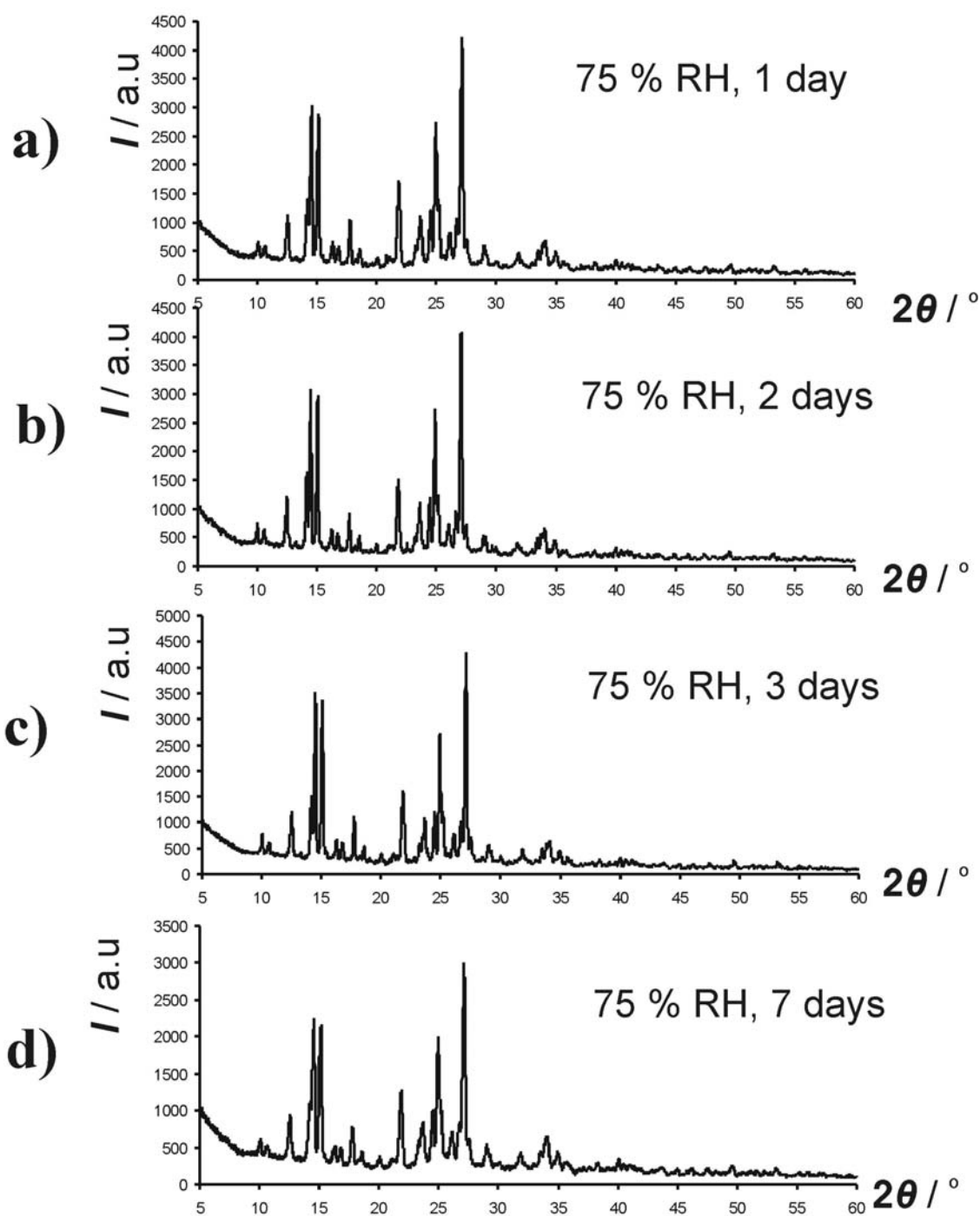


Figure S24. PXRD patterns for the cocrystal of $(\text{tp})_2(\text{DL-ta})$ after exposure to 75% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

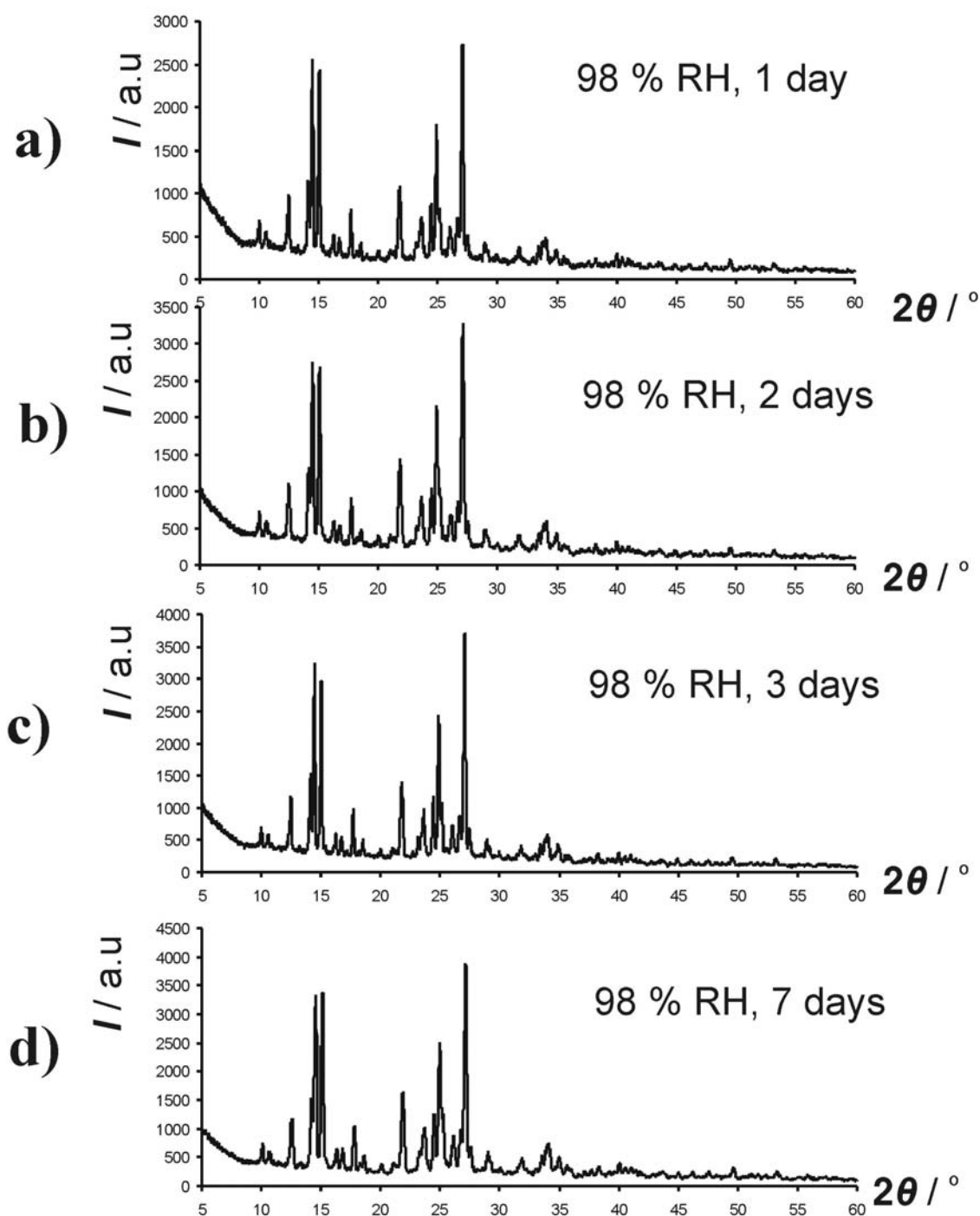


Figure S25. PXRD patterns for the cocrystal of $(tp)_2(DL-ta)$ after exposure to 98% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

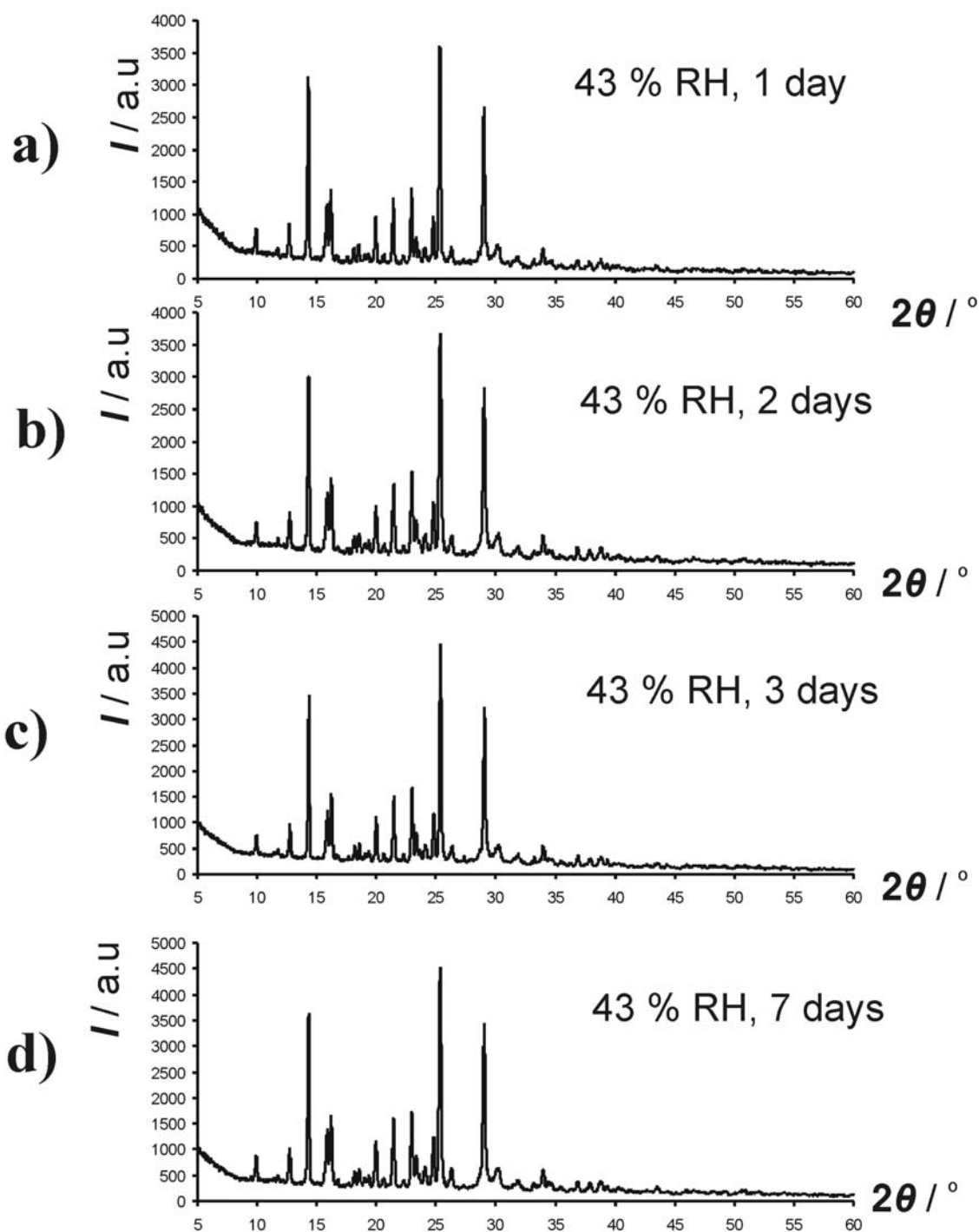


Figure S26. PXRD patterns for the cocrystal of (tp)(D-ma) after exposure to 43% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

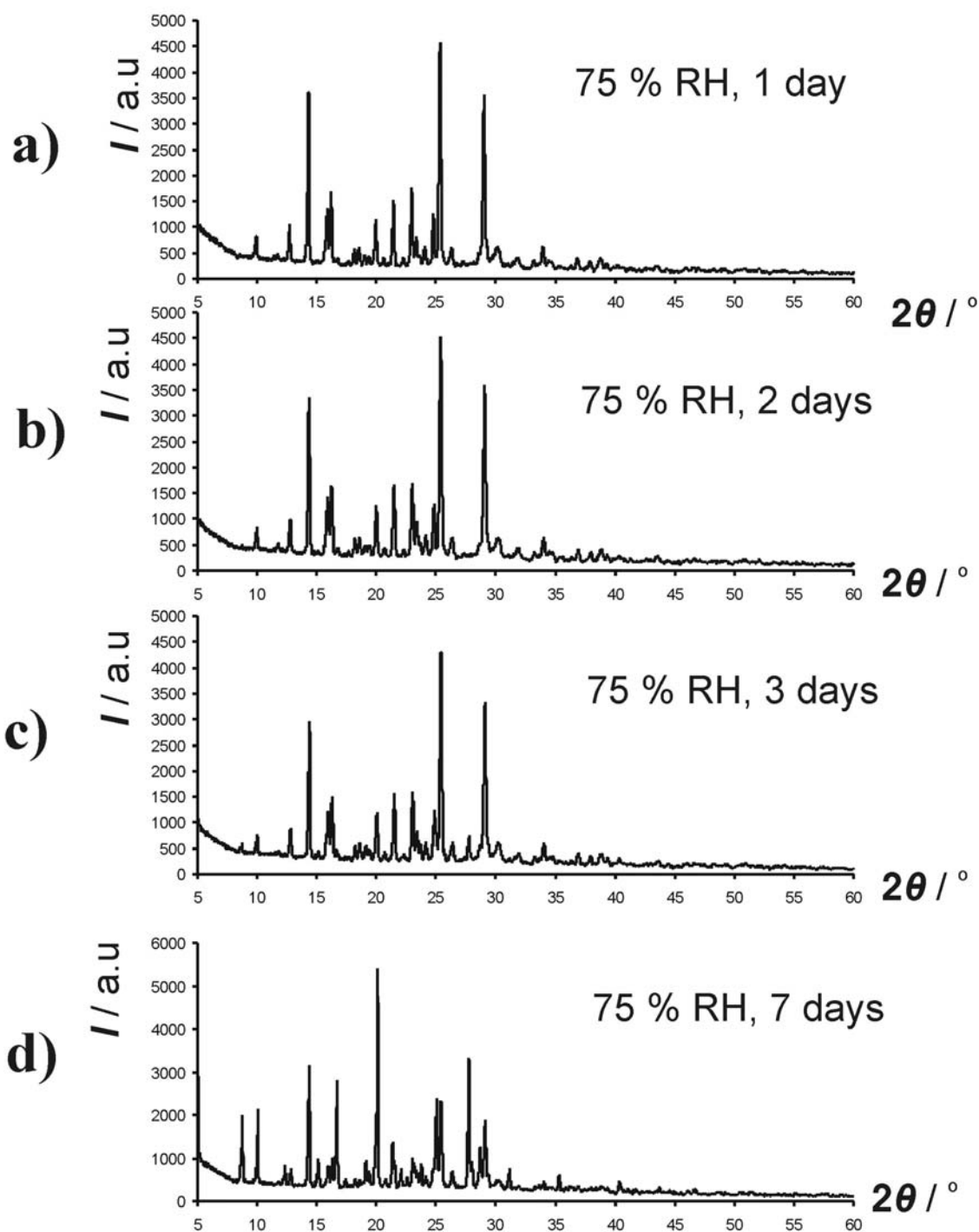


Figure S27. PXRD patterns for the cocrystal of (tp)(D-ma) after exposure to 75% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

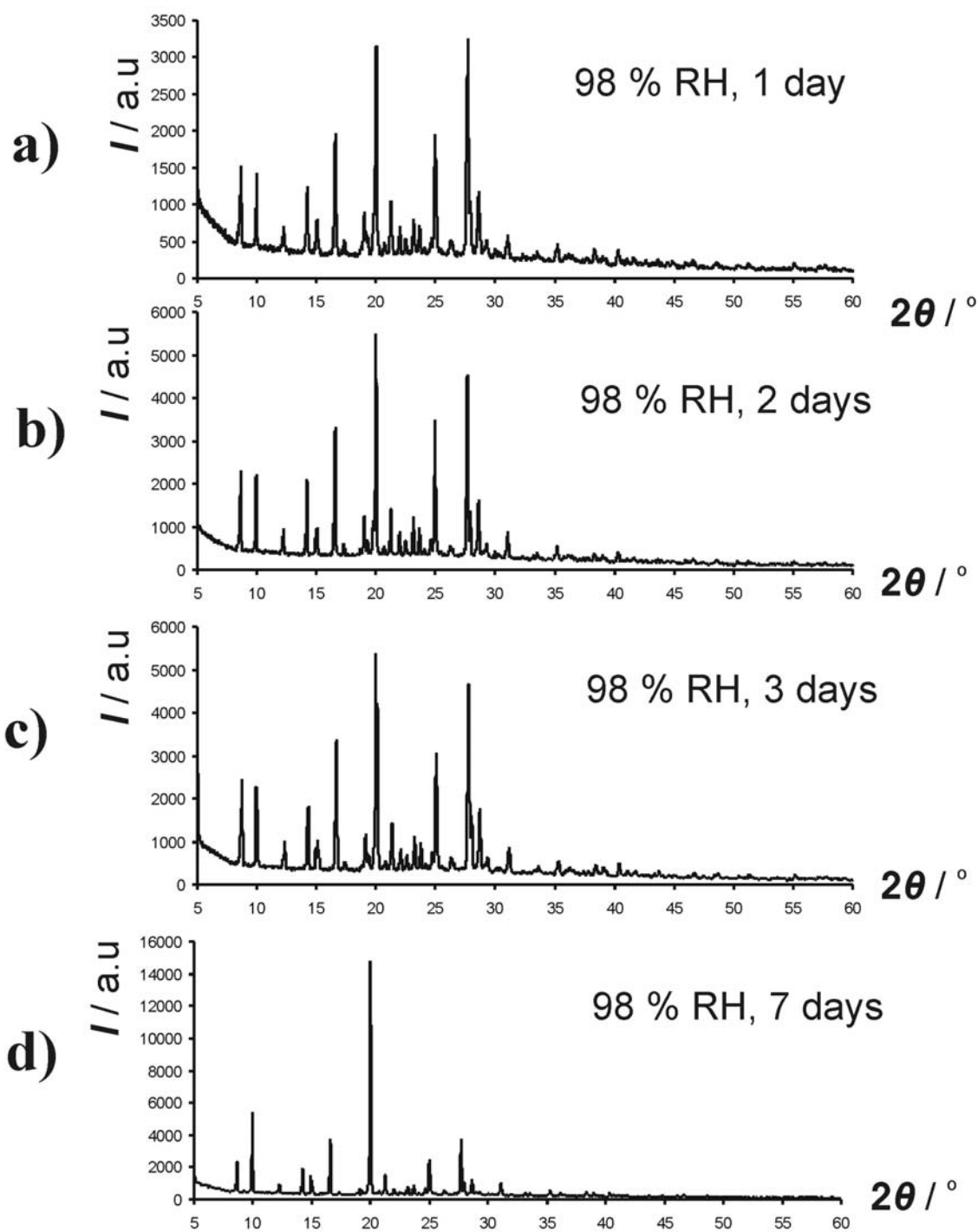


Figure S28. PXRD patterns for the cocrystal of $(tp)(D-ma)$ after exposure to 98% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

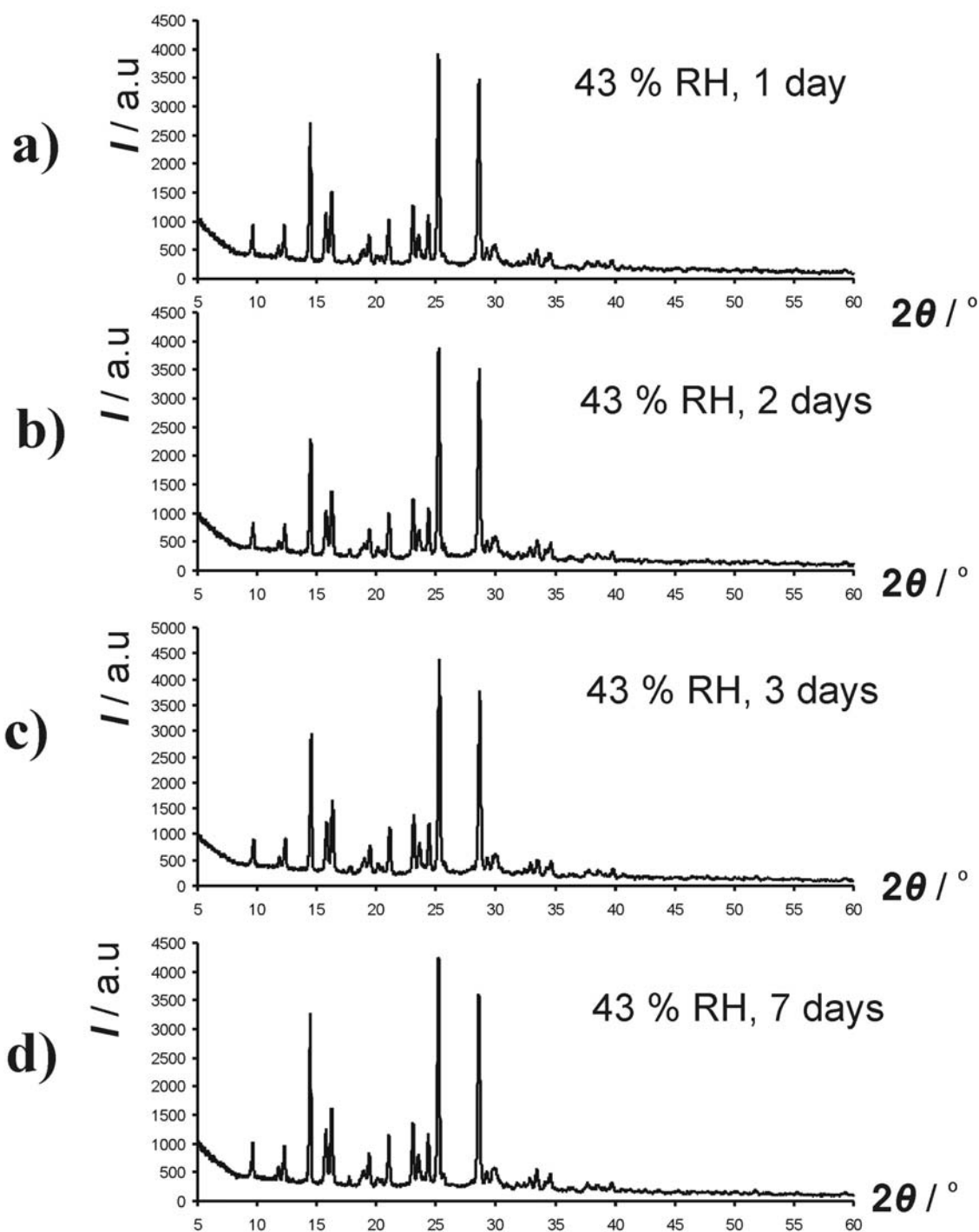


Figure S29. PXRD patterns for the cocrystal of (tp)(DL-ma) after exposure to 43% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

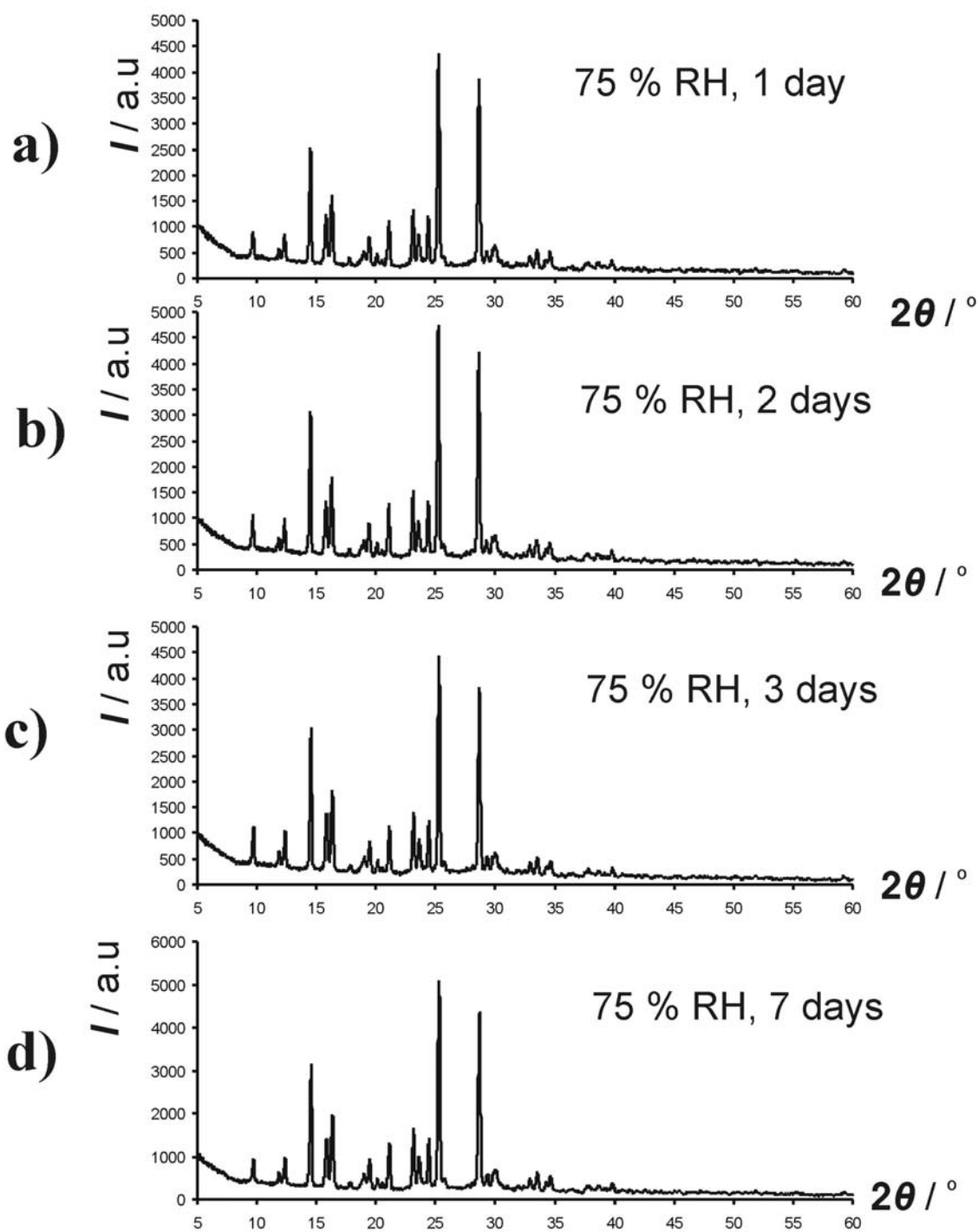


Figure S30. PXRD patterns for the cocrystal of (tp)(DL-ma) after exposure to 75% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

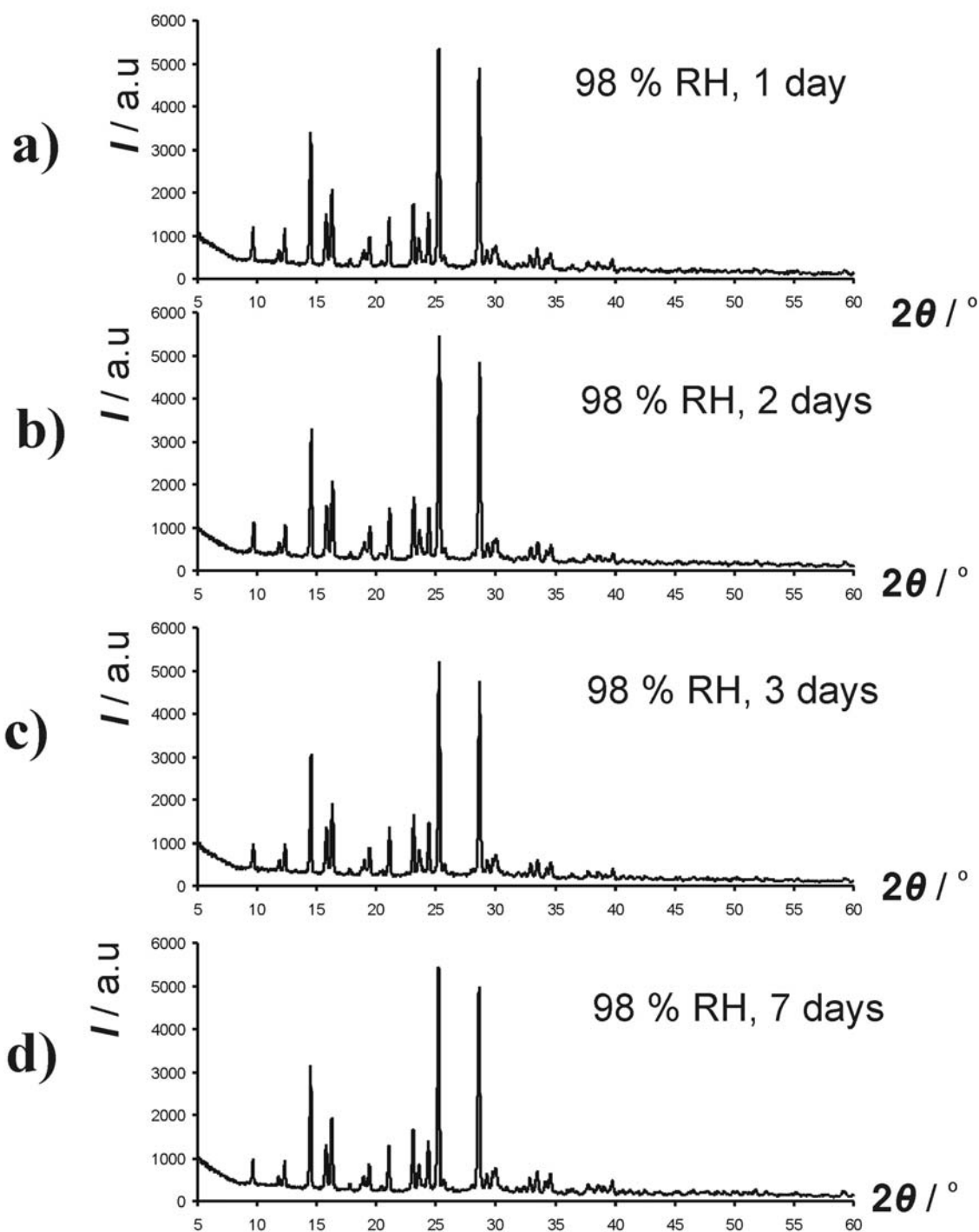


Figure S31. PXRD patterns for the cocrystal of (tp)(DL-ma) after exposure to 98% relative humidity for: a) 1 day; b) 2 days; c) 3 days and d) 7 days.

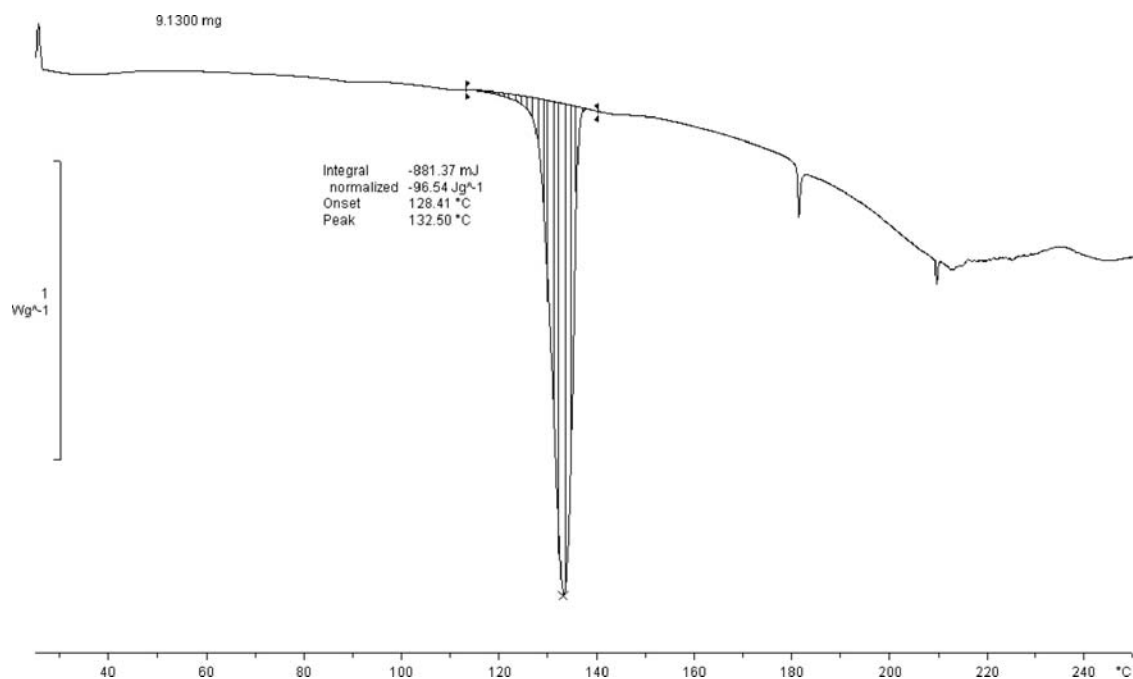


Figure 32. DSC thermogram for the (tp)(D-ma) cocrystal.

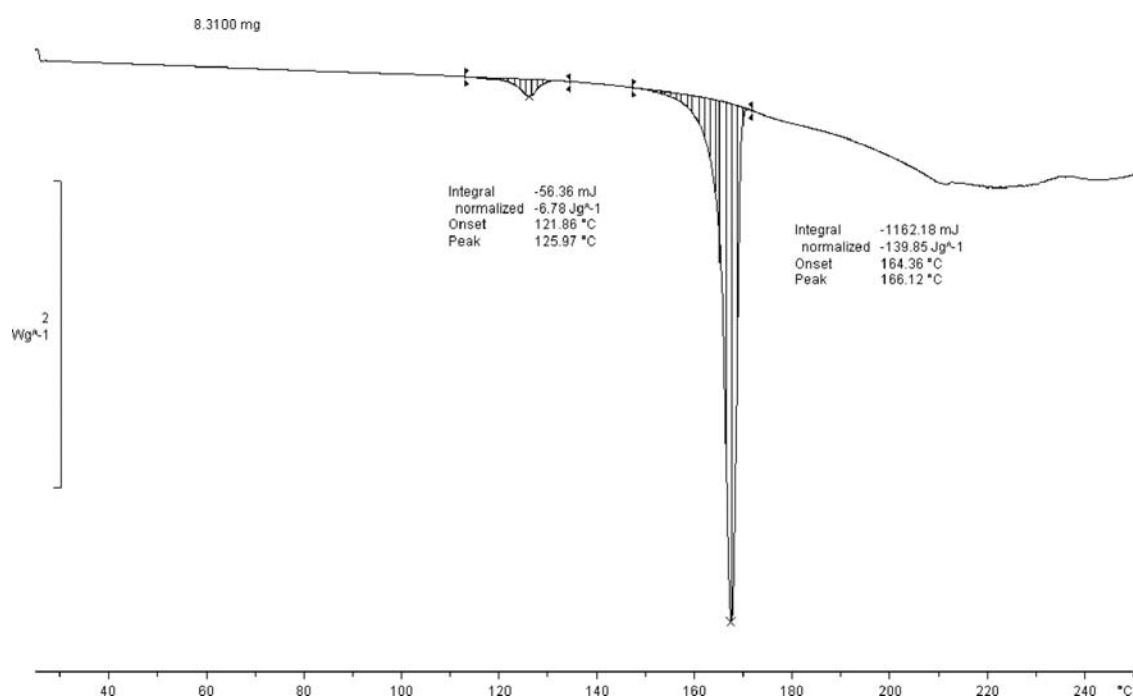


Figure 33. DSC thermogram for the (tp)(DL-ma) cocrystal.

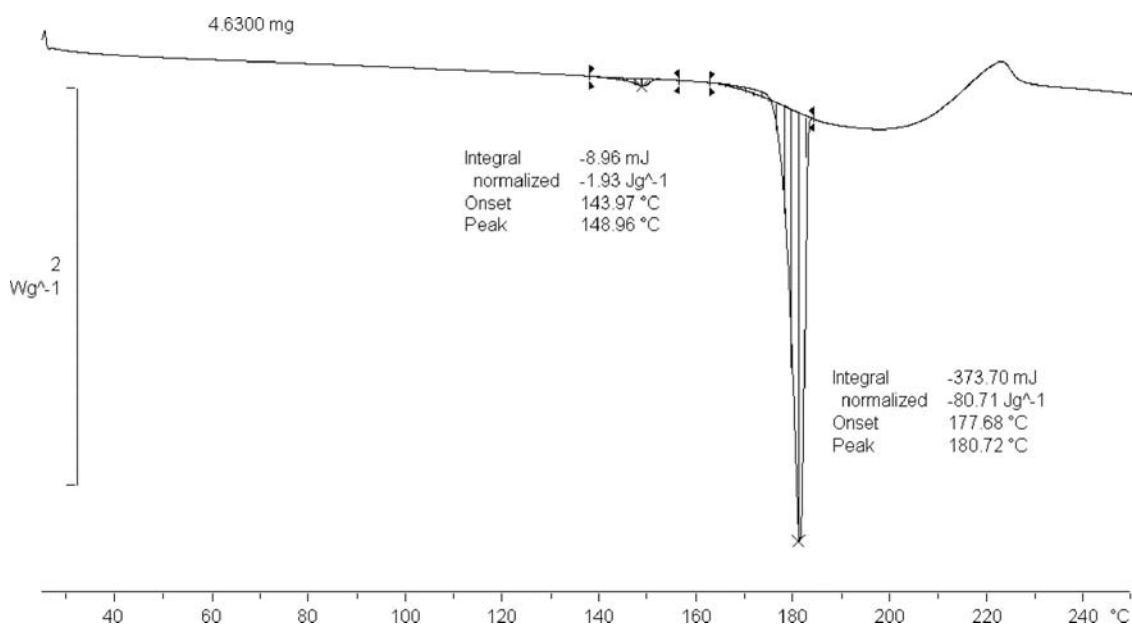


Figure 34. DSC thermogram for the $(tp)_2(D-ta)$ cocrystal.

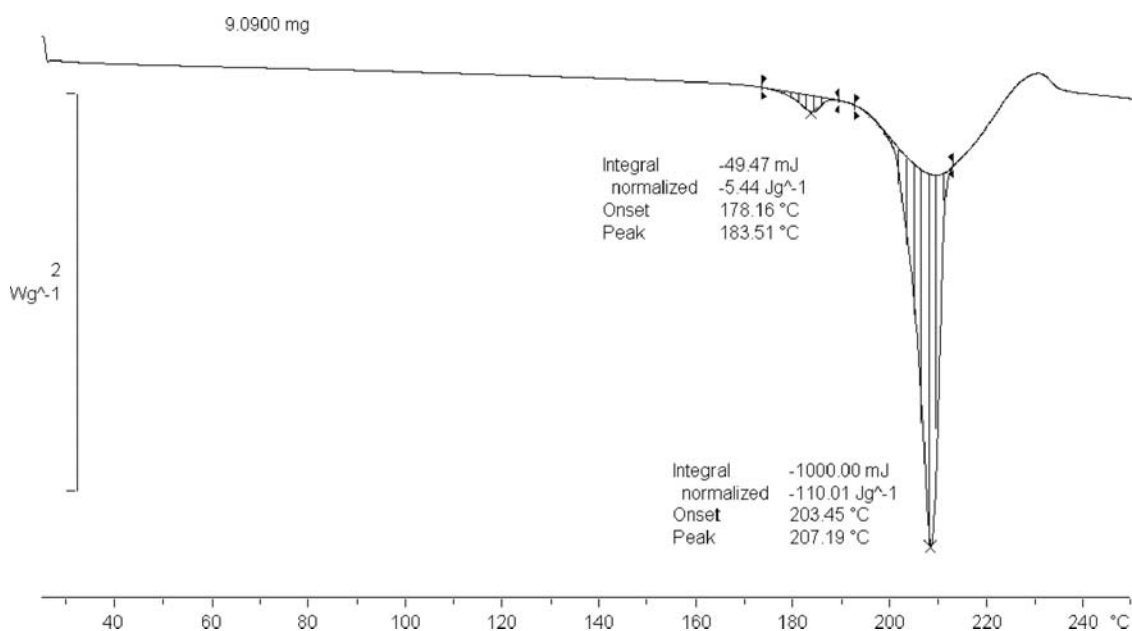


Figure 35. DSC thermogram for the $(tp)_2(DL-ta)$ cocrystal.