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Supporting information for article:

Solvates of selected fenamic acids with substituted pyridines: structure, thermal stability and desolvation

Jacky Bouanga Boudiombo and Ayesha Jacobs

SUPPLEMENTARY DATA

Solvates of selected fenamic acids with substituted pyridines: structure, thermal stability and desolvation

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1.1S Thermal analysis

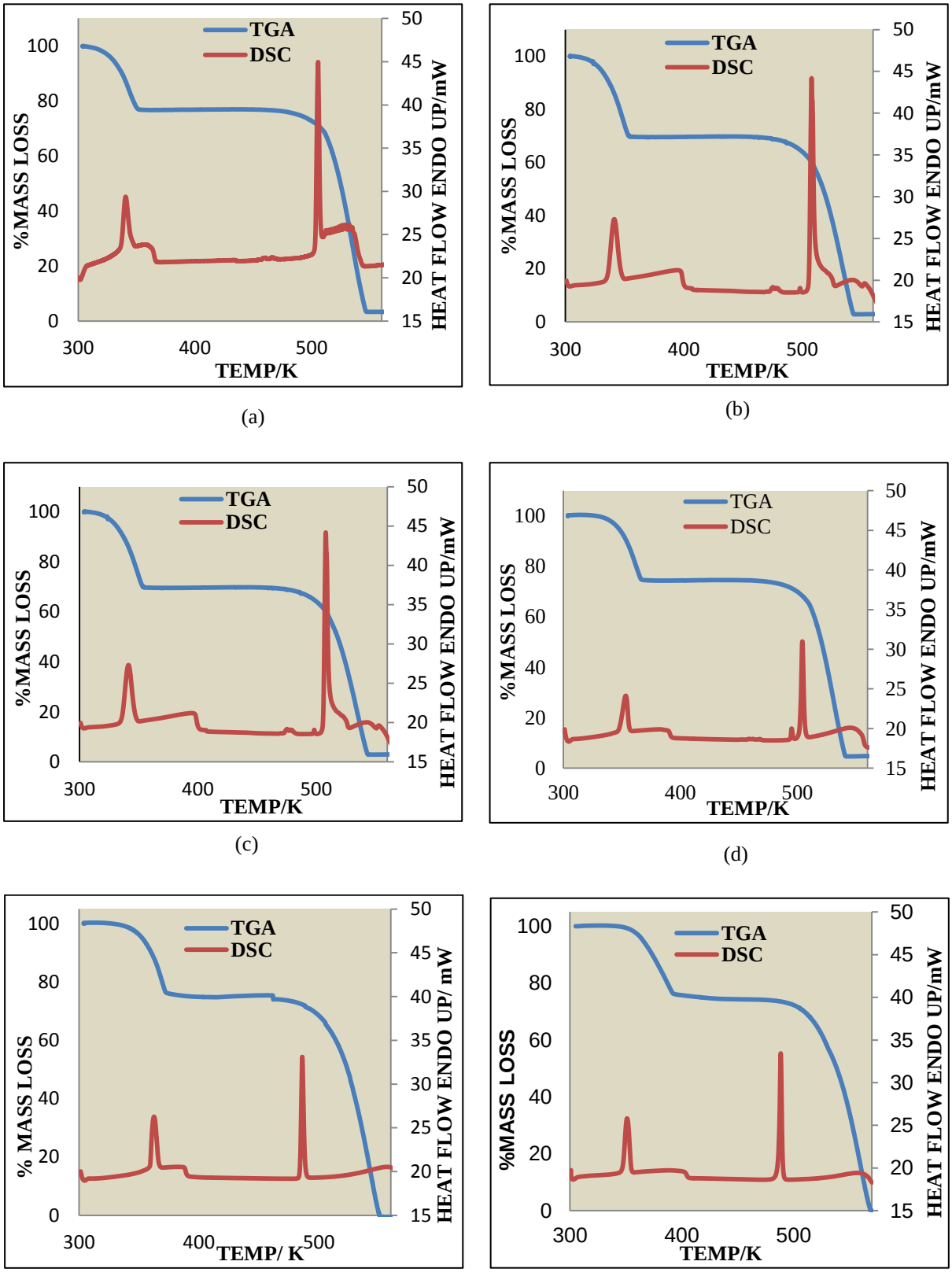


Figure 1S: TGA and DSC curves of (a) MA•2PIC FORM II, (b) MA•3PIC, (c) MA•3ClPYR, (d) MA•4PIC, (e) TFA•2PIC and (f) TFA•3PIC.

1.2S Powder X-ray diffraction (Desolvation experiments)

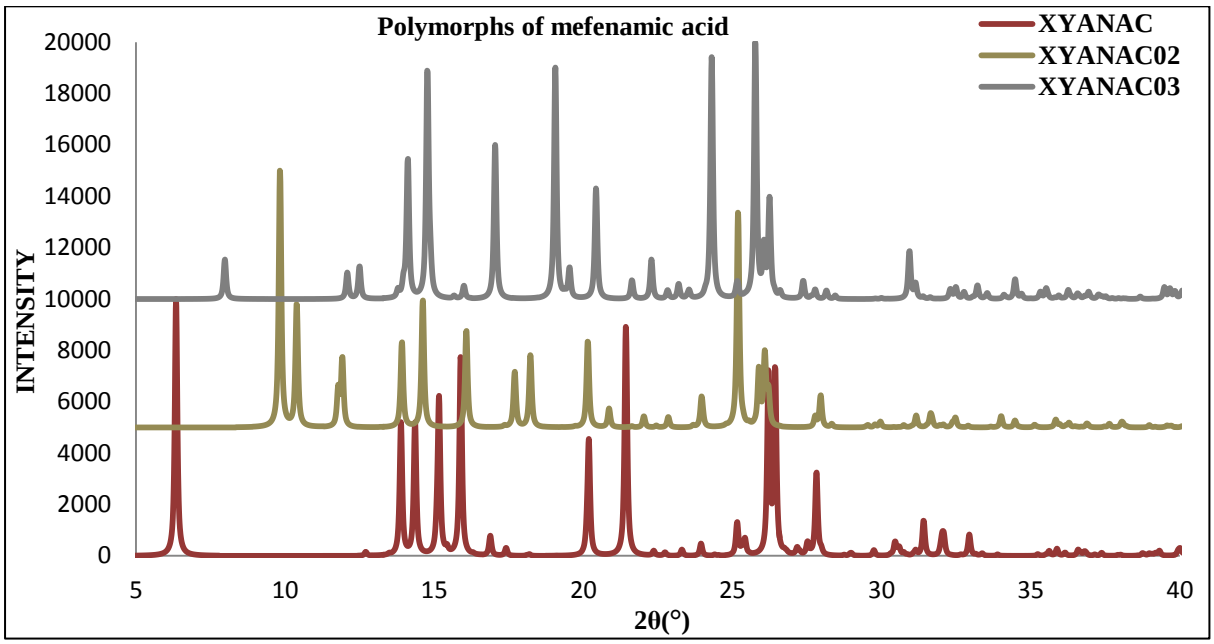


Figure 2S: Simulated PXRD patterns of mefenamic acid polymorphs XYANAC (McConnell et al. 1976), XYANAC02 (Lee et al. 2006) and XYANAC03 (SeethaLekshmi et al. 2012) obtained from Mercury (Macrae et al. 2008), (CSD version 5.37, November 2015, May 2016 update; Groom et al. 2016).

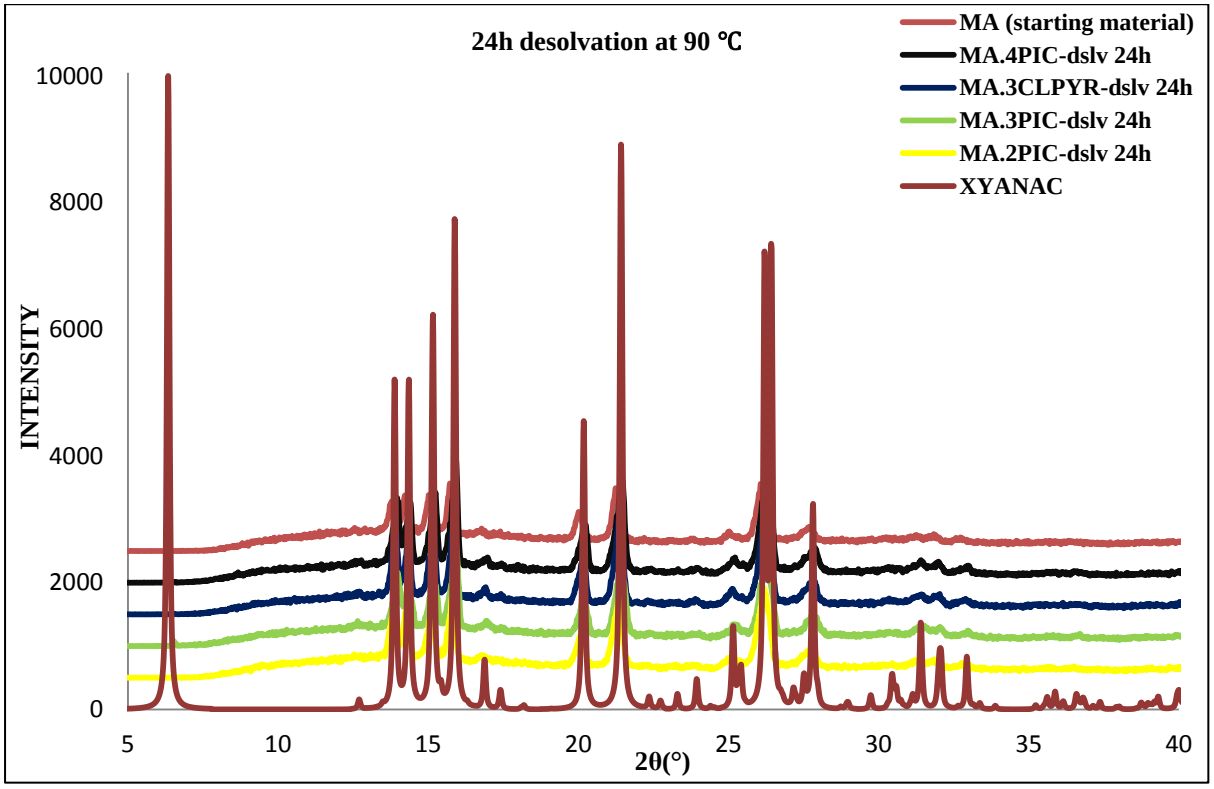


Figure 3S: Patterns obtained from the PXRD analyses of mefenamic acid solvates subjected to 24 h desolvation at 90 °C.

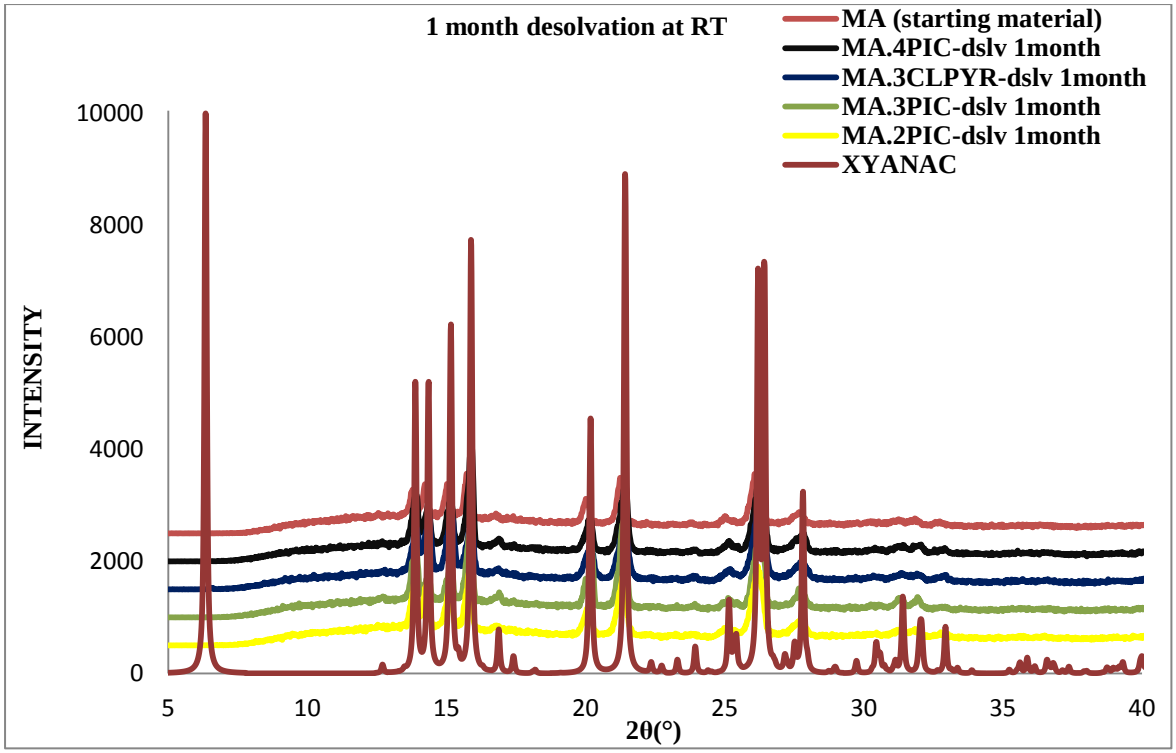


Figure 4S: Patterns obtained from the PXRD analyses of mefenamic acid solvates after one month of desolvation at room temperature (RT).

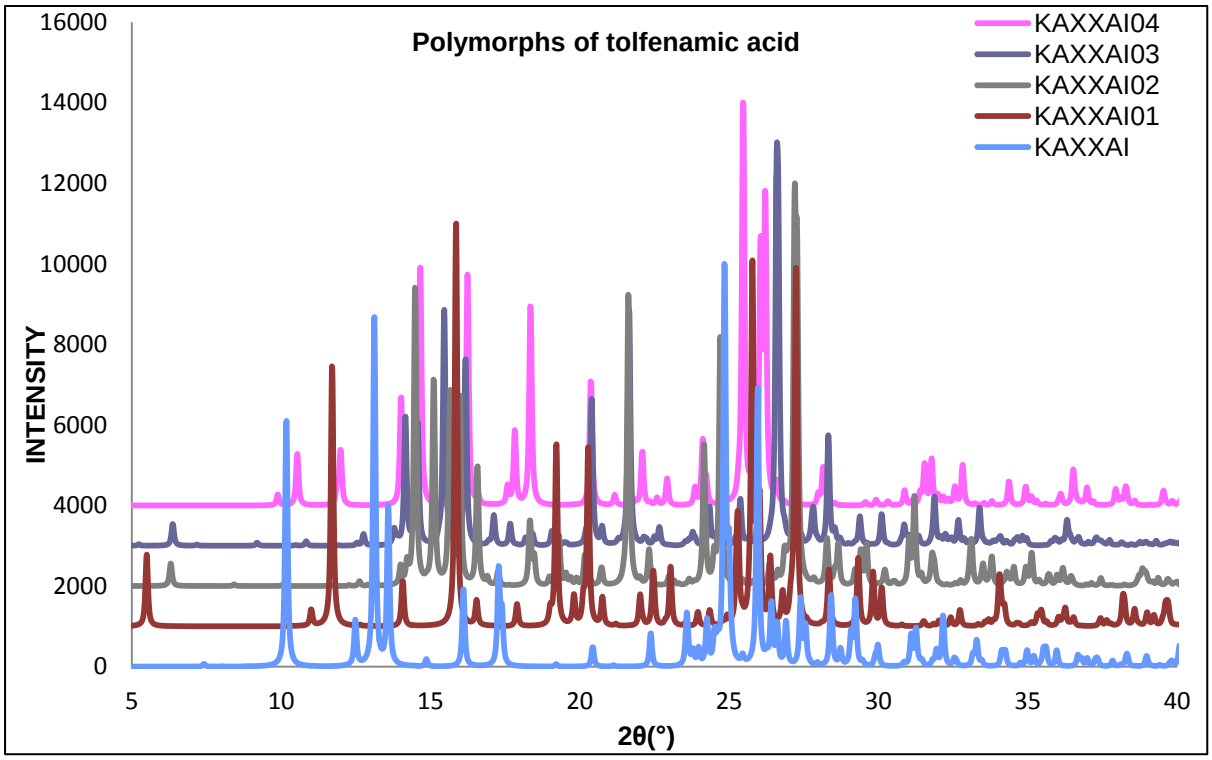


Figure 5S: Simulated PXRD patterns of tolfenamic acid polymorphs KAXXAI, KAXXAI01 (Andersen et al. 1989), KAXXAI02, KAXXAI03 and KAXXAI04 (Lopez-Meijas et al. 2009) obtained from Mercury (CSD version 5.37, November 2015, May 2016 update).

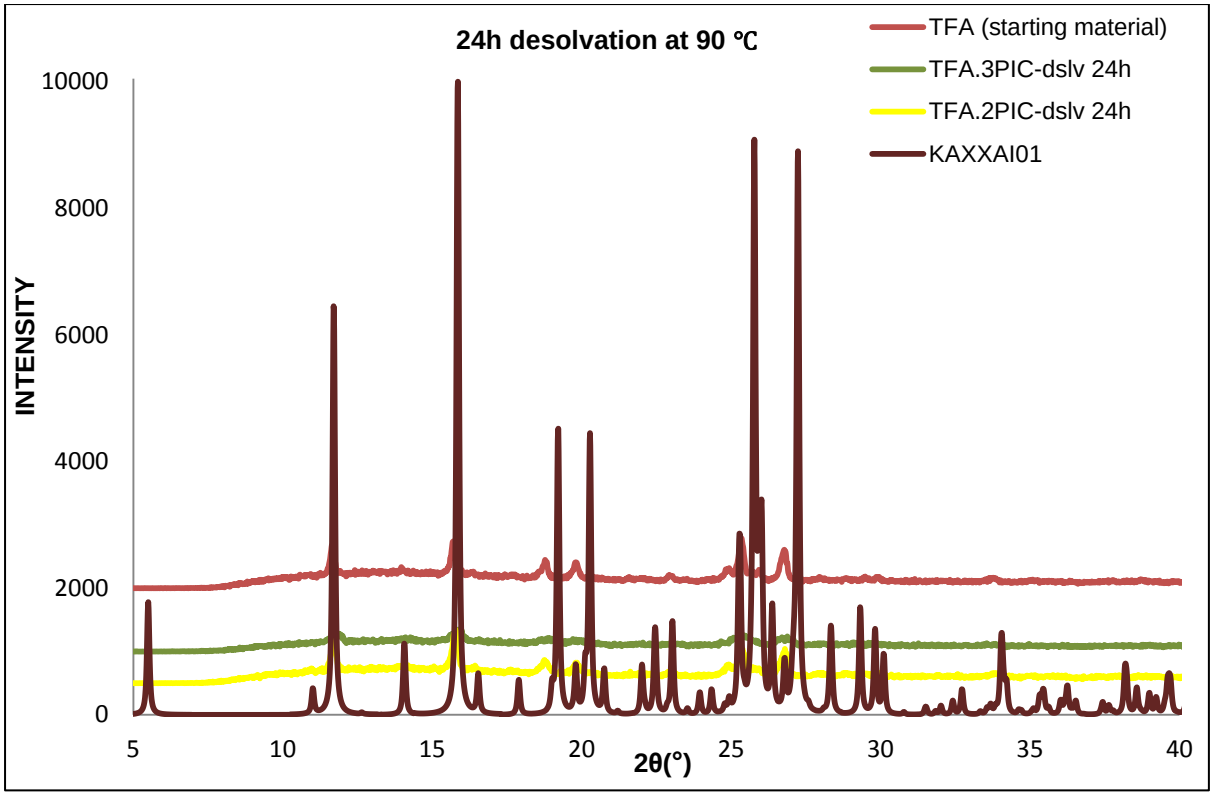


Figure 6S: Patterns obtained from the PXRD analyses of tolfenamic acid solvates after 24h desolvation at 90 °C.

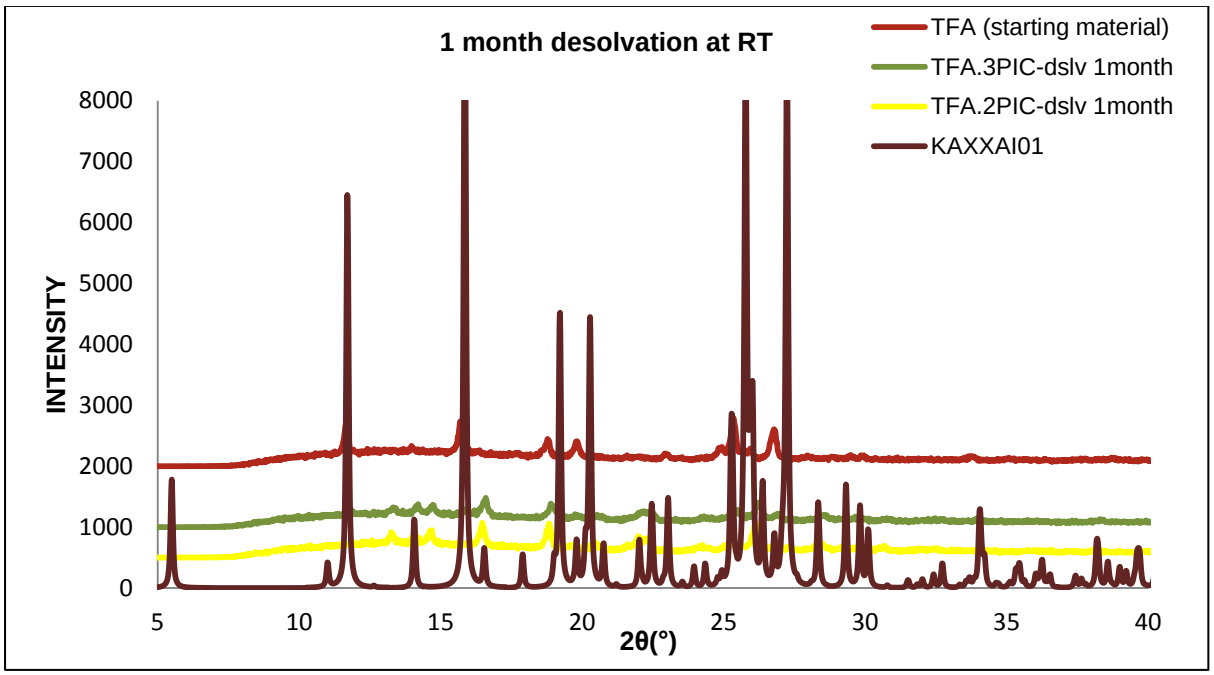


Figure 7S: Patterns obtained from the PXRD analyses of tolfenamic acid solvates with pyridines after one month of desolvation at RT.

1.3S Kinetics of desolvation plots

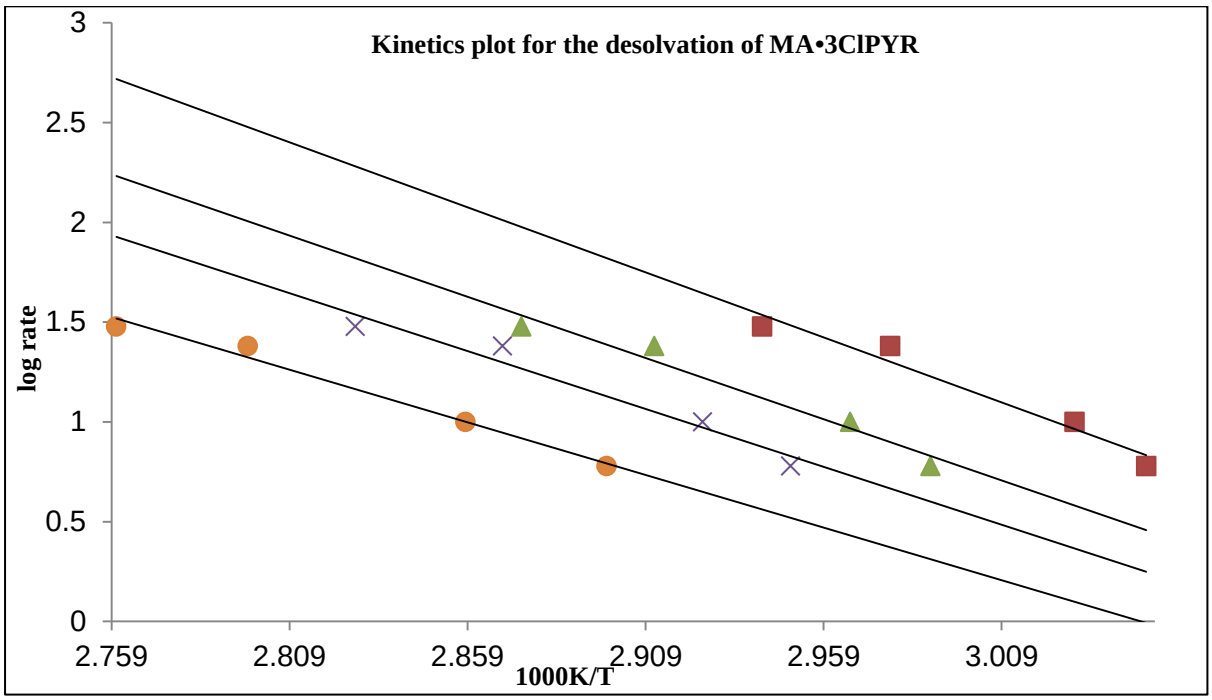


Figure 8S: Log rate vs. 1/T graphs obtained for the desolvation of MA•3ClPYR.

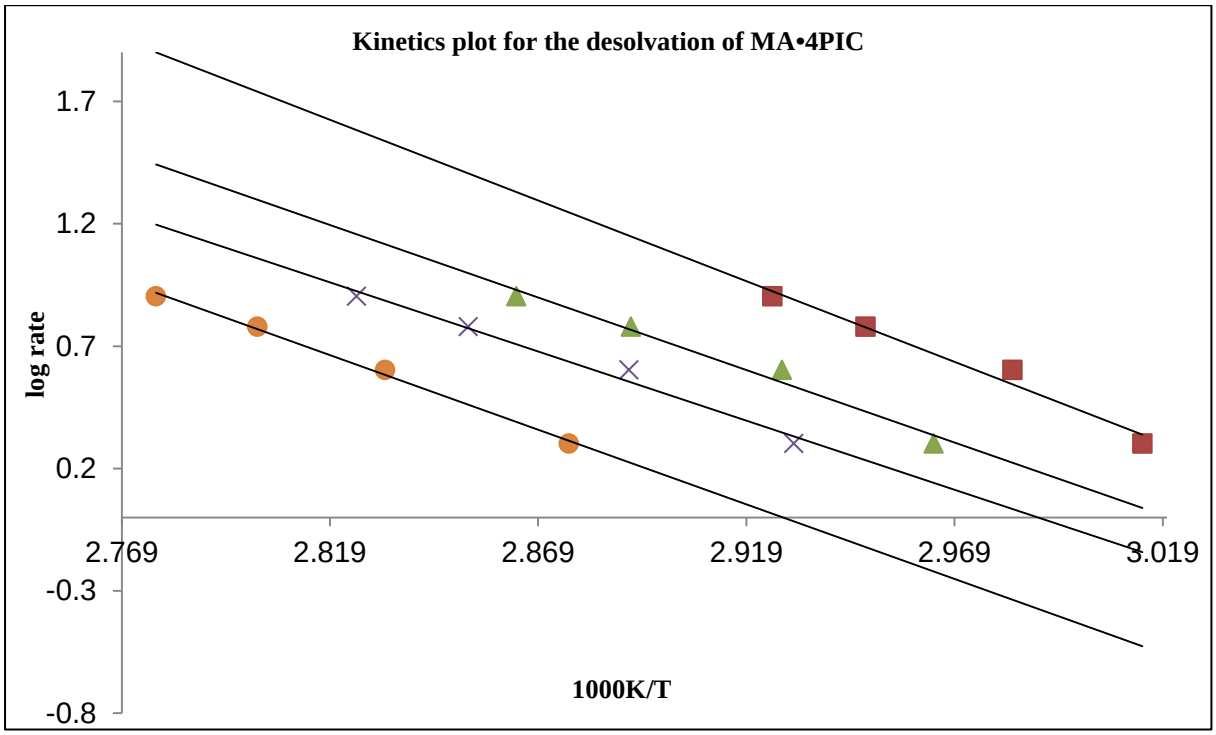


Figure 9S: Log rate vs. 1/T graphs obtained for the desolvation of MA•4PIC.

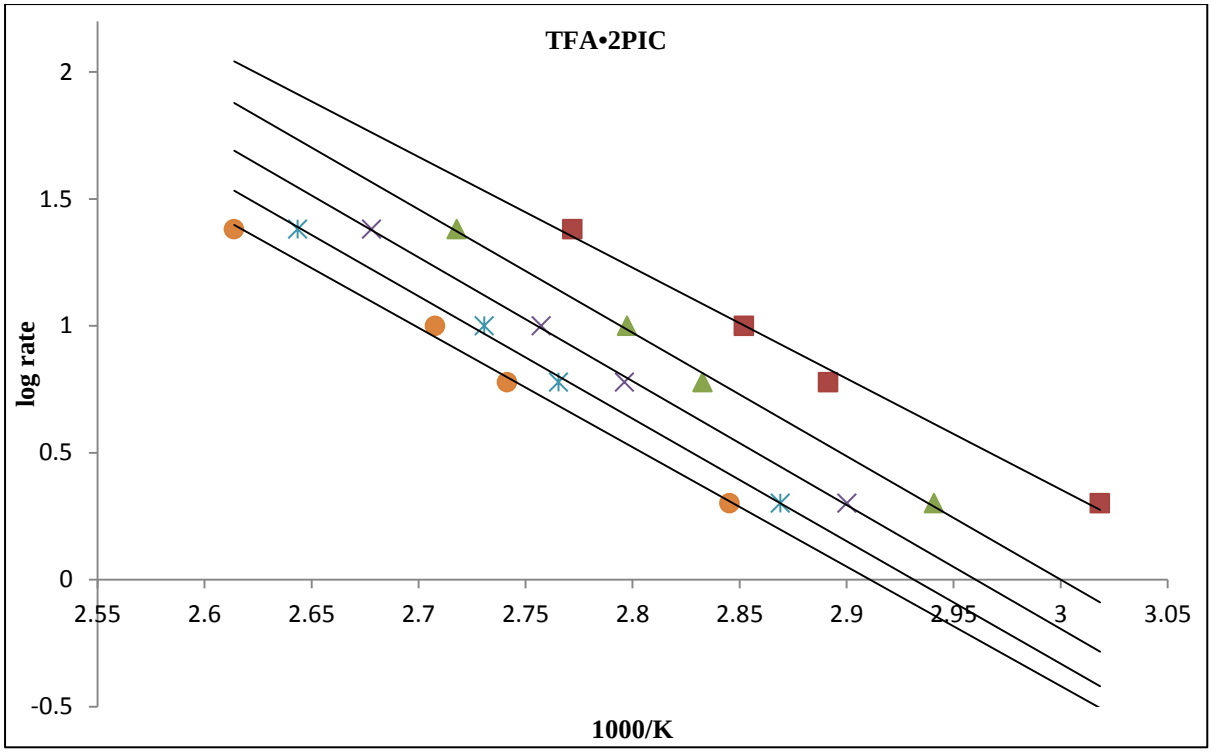


Figure 10S: Log rate vs. 1/T graphs obtained for the desolvation of TFA•2PIC.

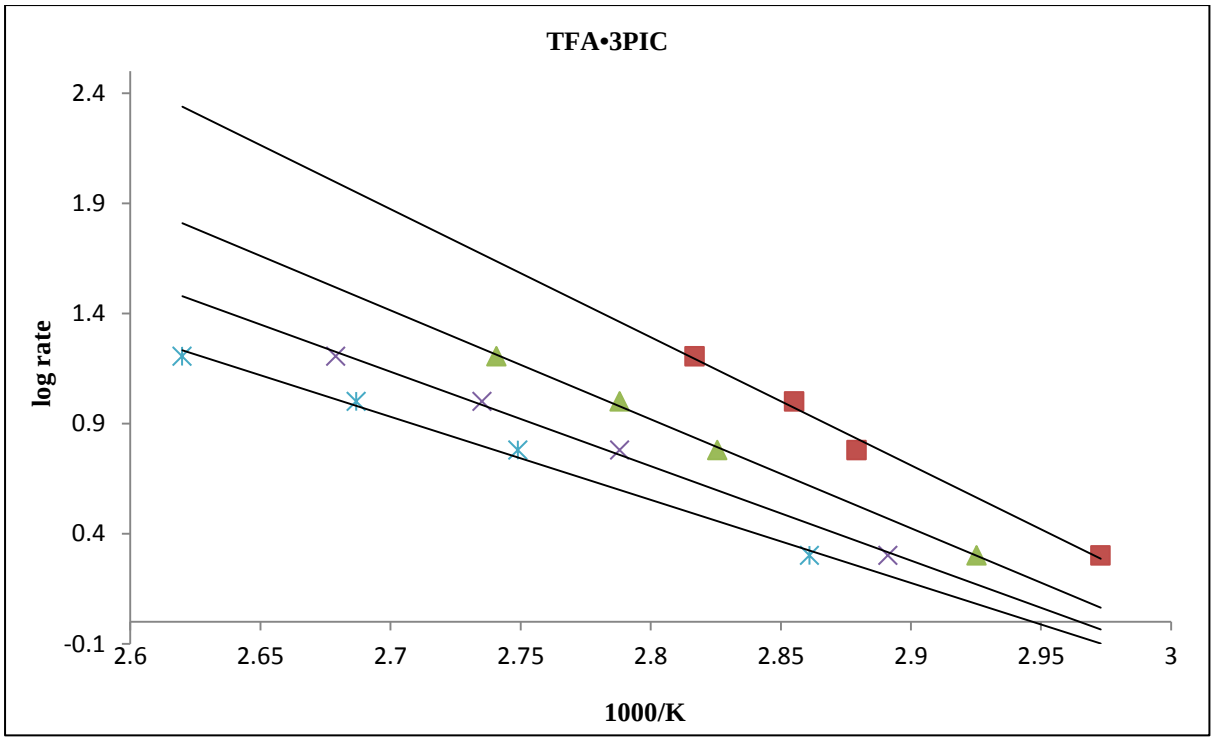


Figure 11S: Log rate vs. 1/T graphs obtained for the desolvation of TFA•3PIC.

1.4S Powder X-ray diffraction (grinding and slurry experiments)

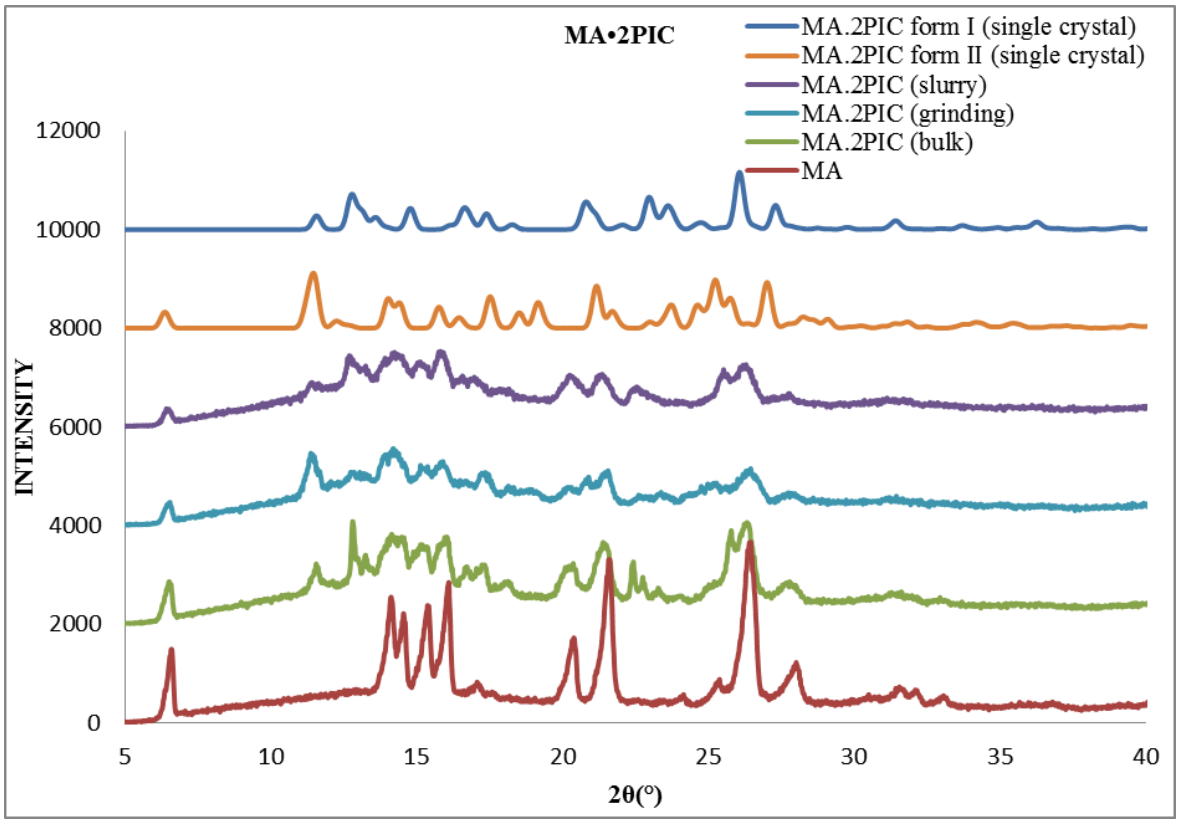


Figure 12S PXRD analyses of MA•2PIC calculated pattern obtained from LAZYPULVERIX (Yvon et al. 1997) of Form I (orange) and Form II (blue), slurry experiment (light blue); grinding experiment (purple), bulk sample (green) and starting material MA (red).

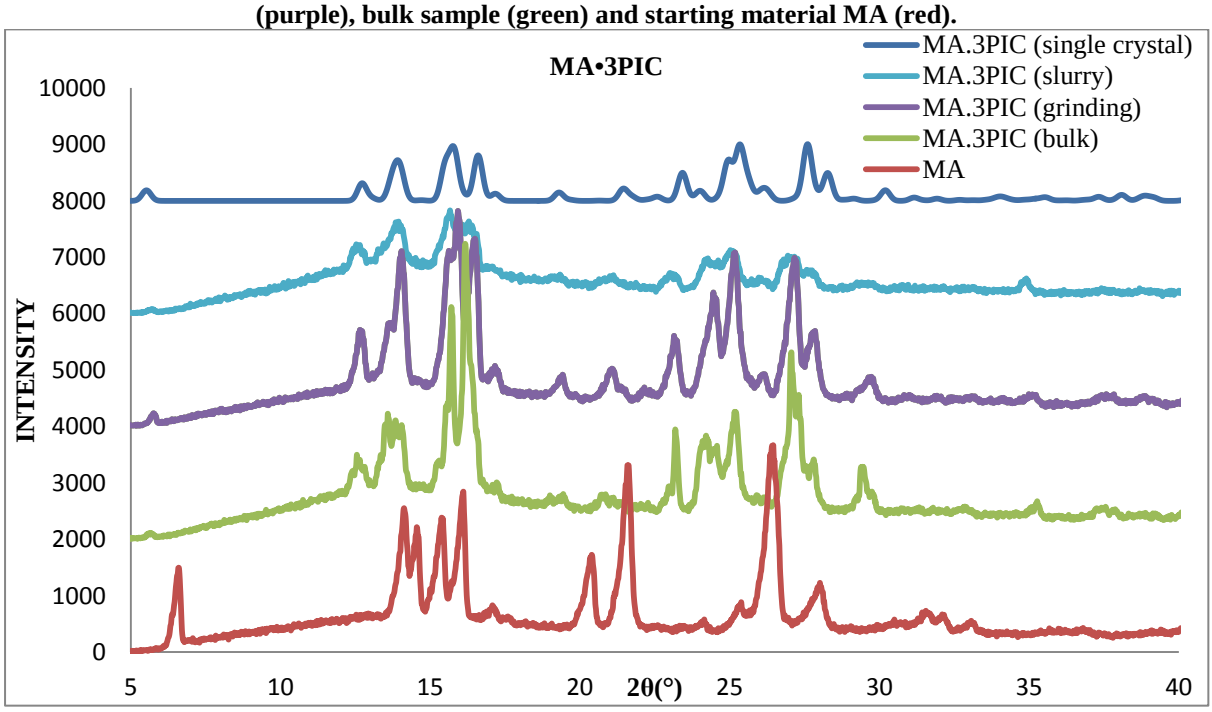


Figure 13S: PXRD analyses of MA•3PIC: calculated pattern obtained from LAZYPULVERIX (blue), and patterns from the slurry experiment (light blue); the grinding experiment (purple), bulk sample (green) and starting material MA (red).

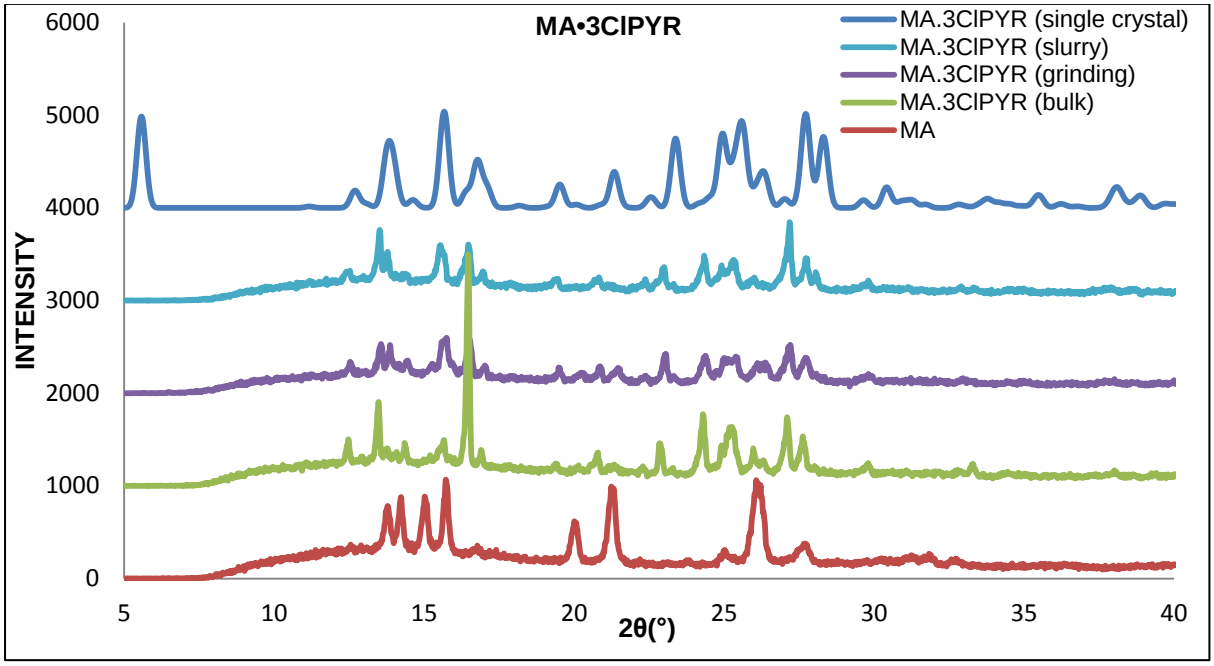


Figure 14S: PXRD analyses of MA•3ClPYR: calculated pattern obtained from LAZYPULVERIX (blue), and patterns from the slurry experiment (light blue); the grinding experiment (purple), bulk sample (green) and starting material MA (red).

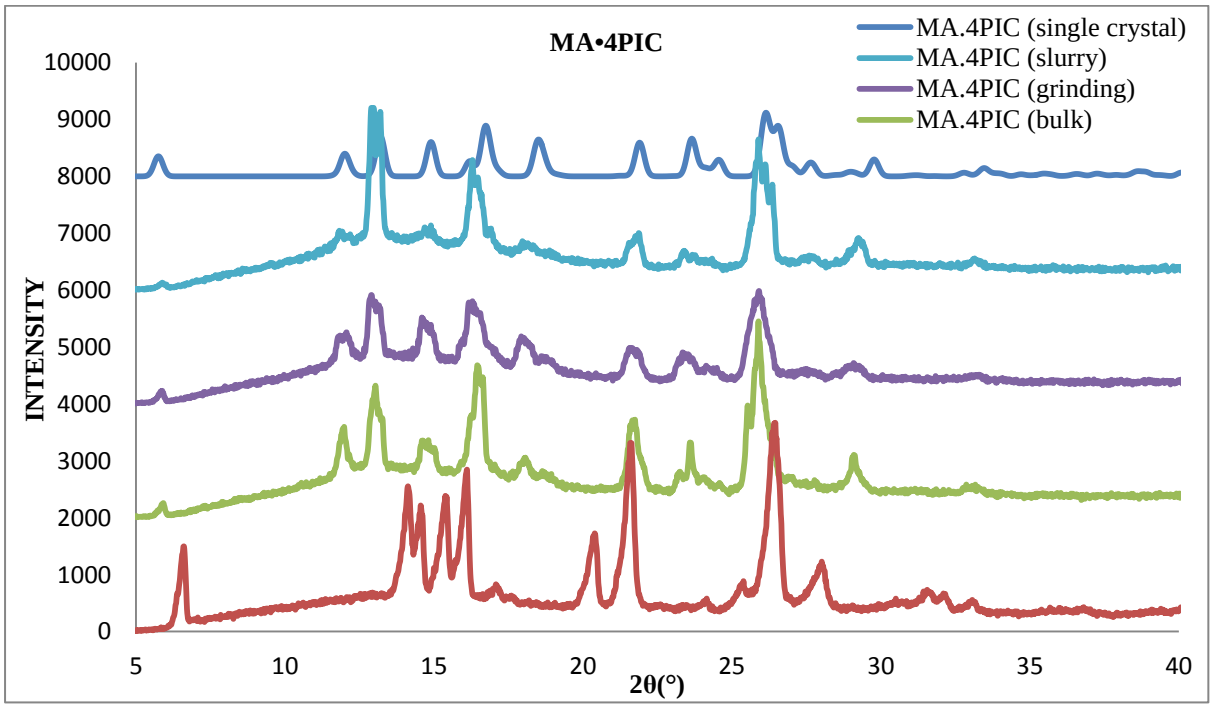
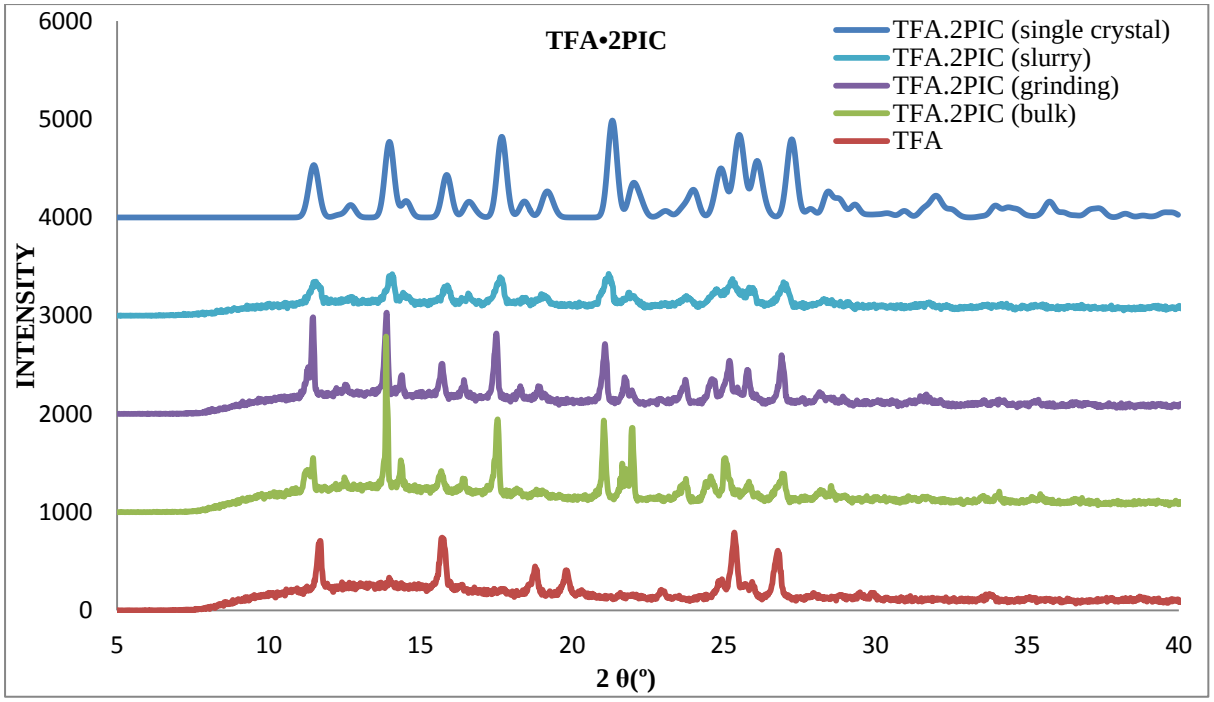


Figure 15S: PXRD analyses of MA•4PIC calculated pattern obtained from LAZYPULVERIX (blue), and patterns from the slurry experiment (light blue); the grinding experiment (purple), bulk sample (green) and starting material MA (red).



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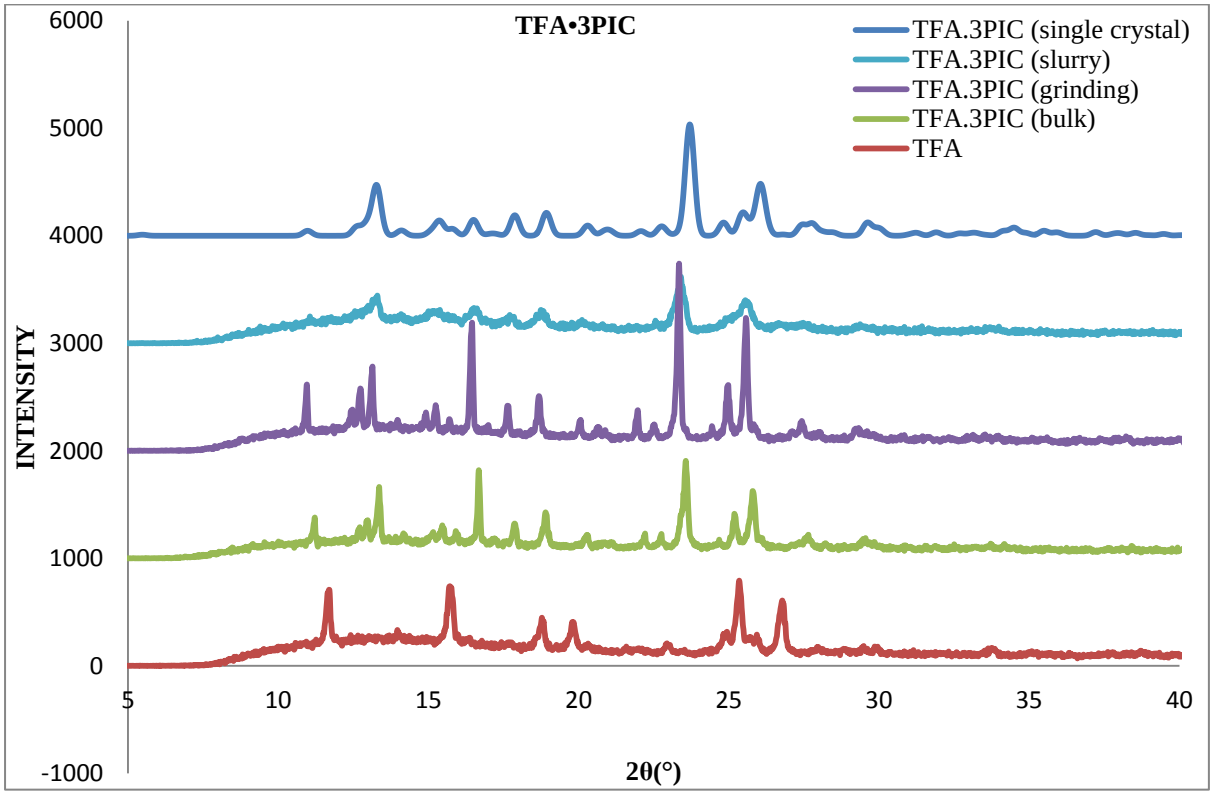

Figure 17S: PXRD analyses of TFA•3PIC: calculated pattern obtained from a LAZYPULVERIX (blue),and patterns from the slurry experiment (light blue); the grinding experiment (purple), bulk sample (green) and starting material TFA (red).

1.5S References

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