Preparation of Pyrazinamide Eutectics versus Cocrystals Based on Supramolecular Synthon Variations

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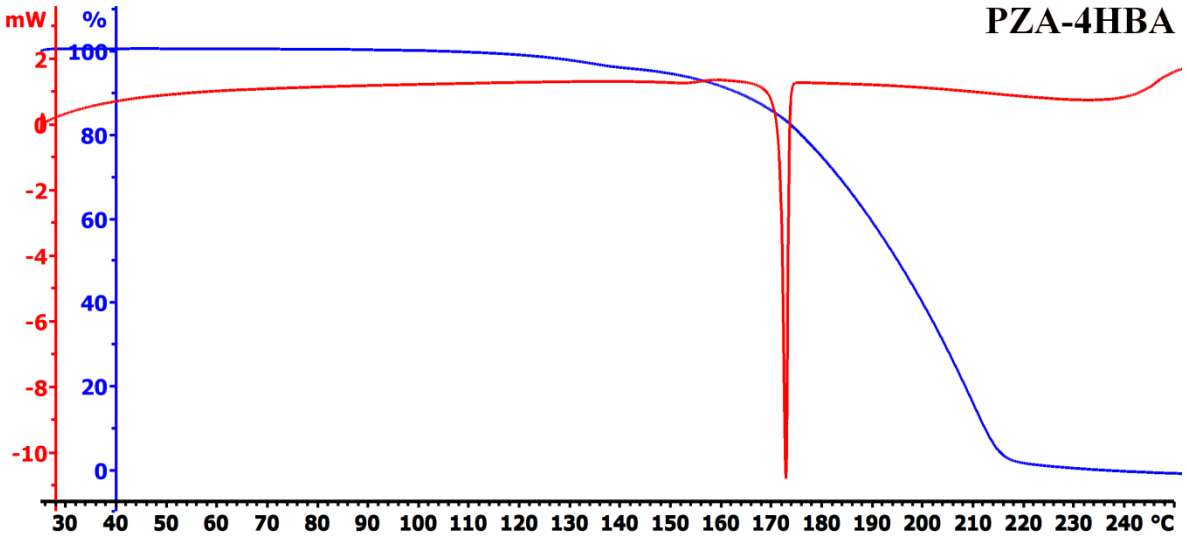
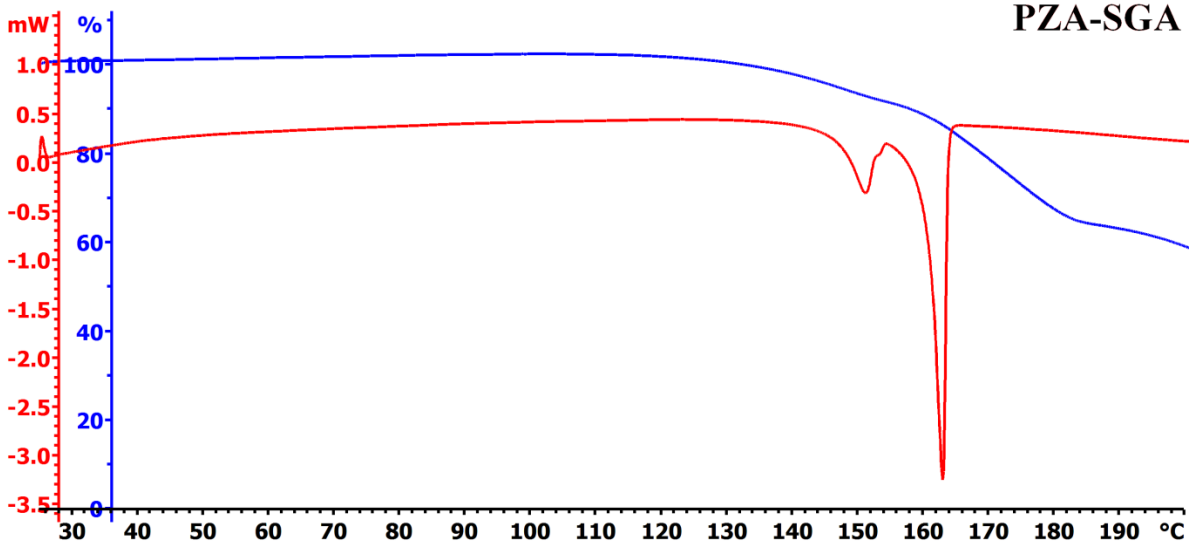


(a)



(b)

Figure S1. DSC (red) and TGA (blue) thermograms of (a) PZA–4HBA and (b) PZA–SGA cocrystals show no phase transition and corresponding weight loss pertaining to solvent incorporation before the melting endotherm indicating that the combinations are non-solvated cocrystals. The cocrystals (PZA–4HBA 172 °C, PZA–SGA 162 °C) have melting point less than their respective parent components (PZA 190 °C, 4HBA 213 °C, SGA 205 °C).

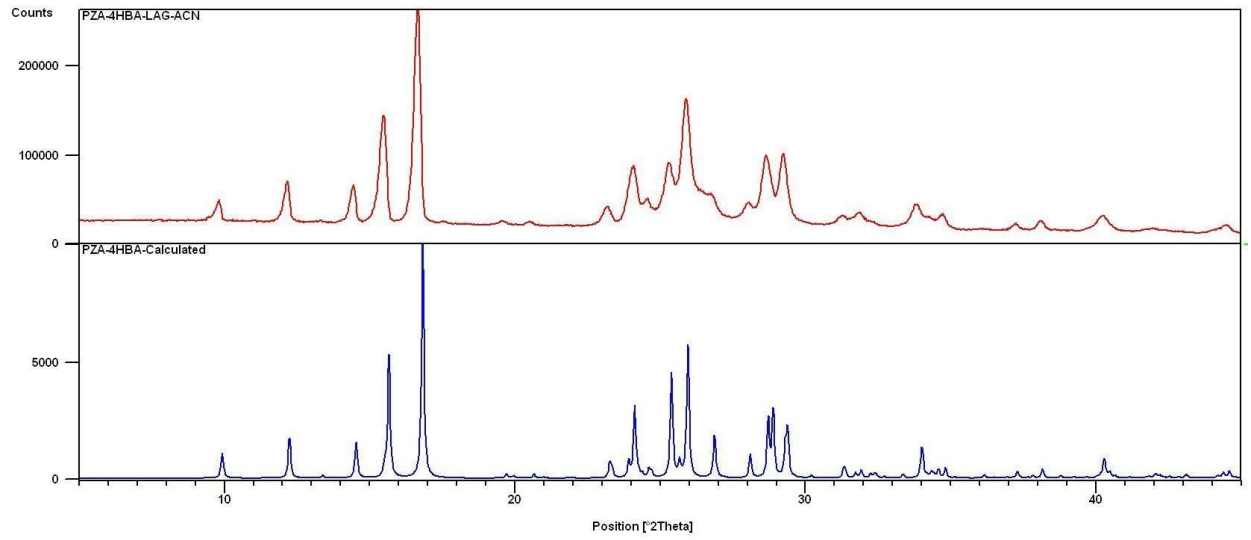
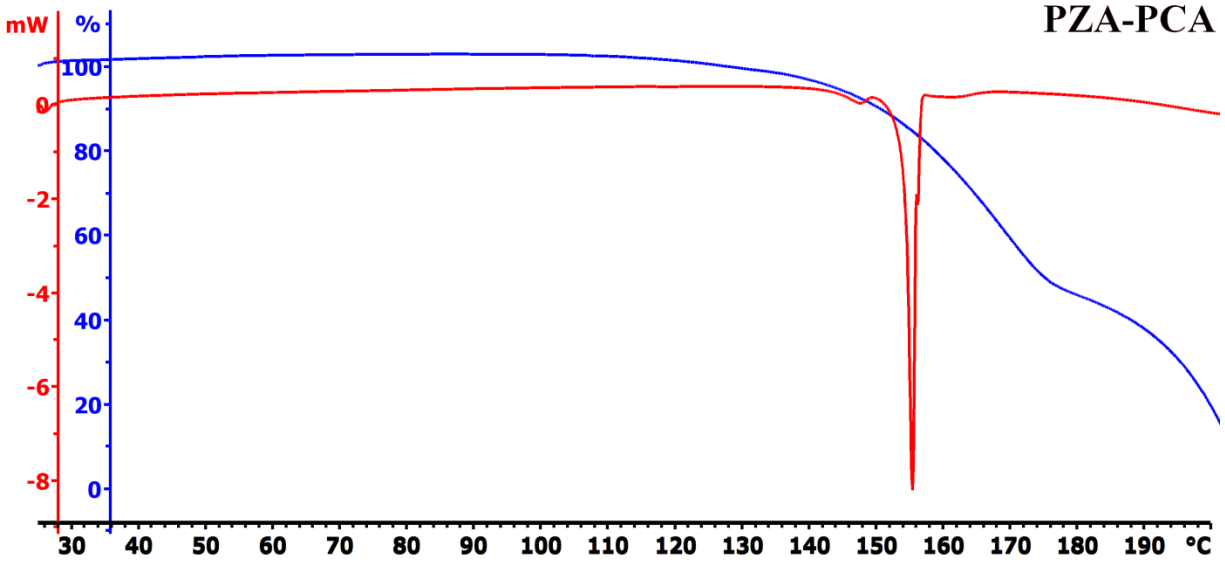
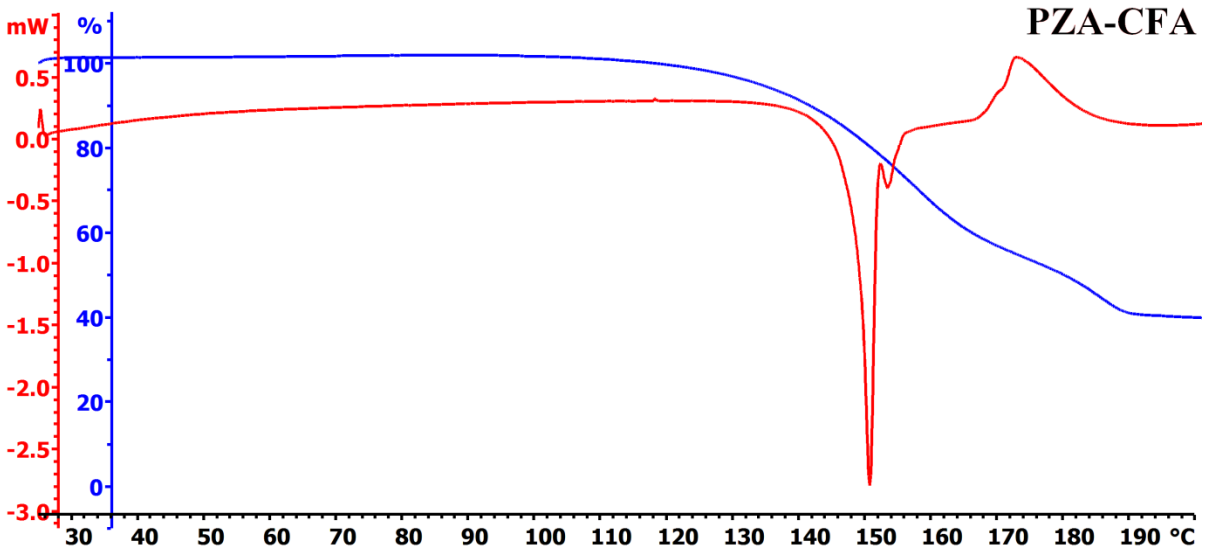


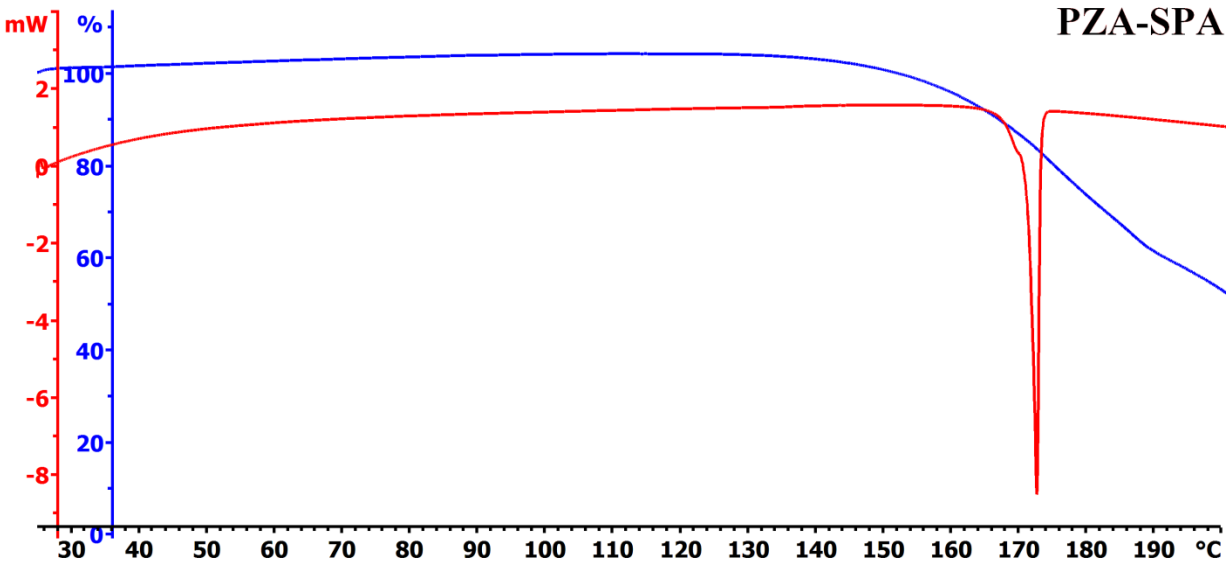
Figure S2. Experimental PXRD pattern (top) of PZA–4HBA cocrystal prepared using LAG shows complete match with that of the calculated powder pattern (bottom) obtained from the X-ray crystal structure.



(a)



(b)



(c)

Figure S3. DSC (red) and TGA (blue) thermograms of (a) PZA–PCA, (b) PZA–CFA and (c) PZA–SPA cocrystals show no phase transition and corresponding weight loss pertaining to solvent incorporation before the melting endotherm indicating that the combinations are non-solvated cocrystals. The cocrystals (PZA–PCA 154 °C, PZA–CFA 150 °C, PZA–SPA 172 °C) have melting point less than their respective parent components (PZA 190 °C, PCA 214 °C, CFA 211 °C, SPA 202 °C).

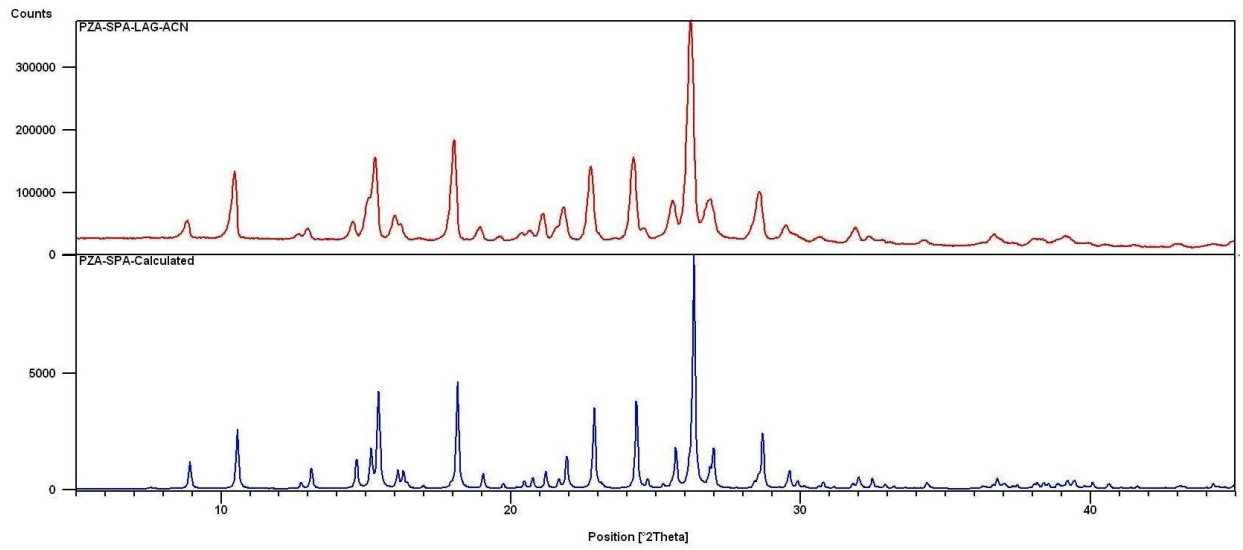


Figure S4. Experimental PXRD pattern (top) of PZA−SPA cocrystal prepared using LAG shows complete match with that of the calculated powder pattern (bottom) obtained from the X-ray crystal structure.

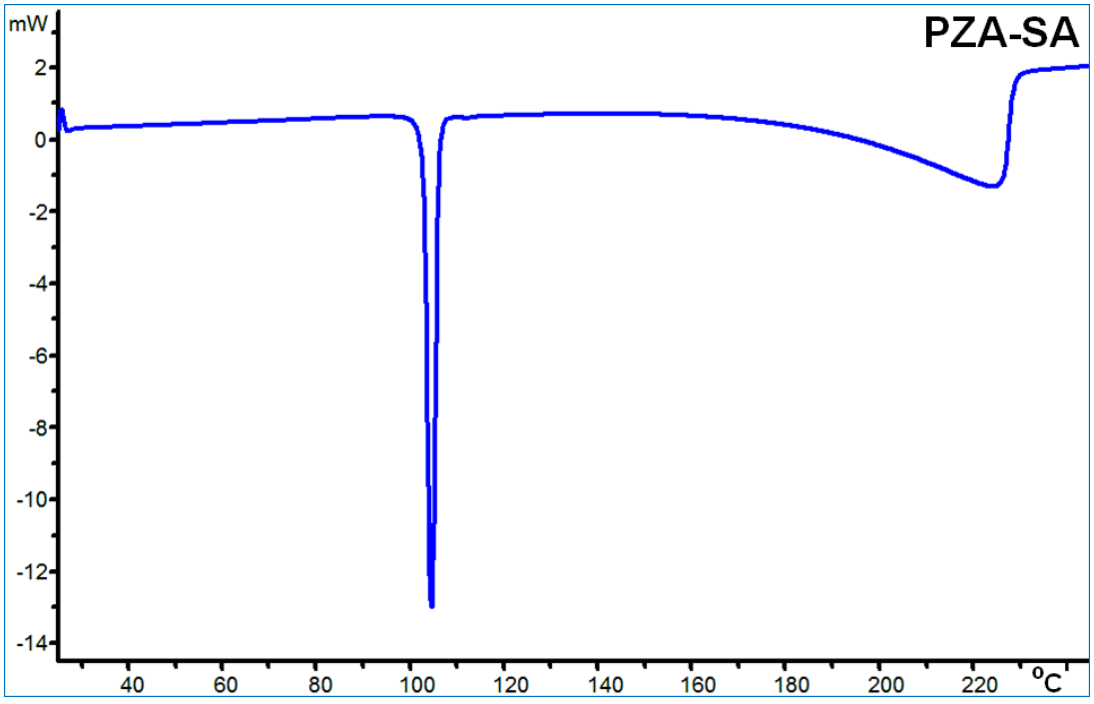
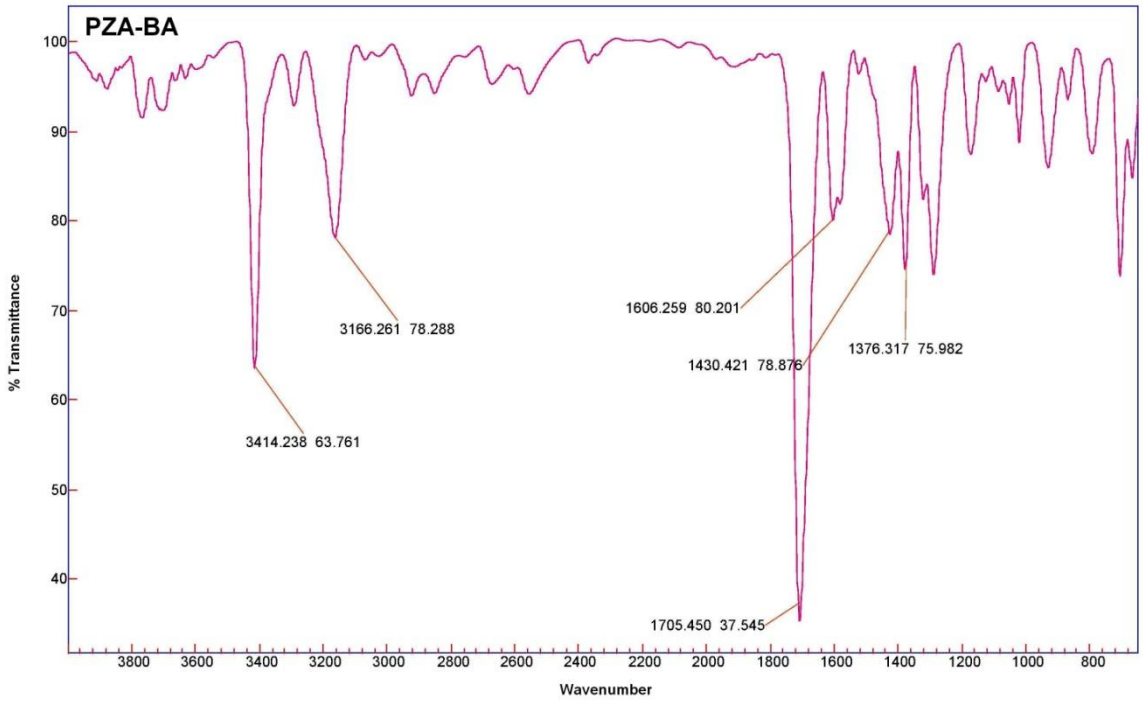
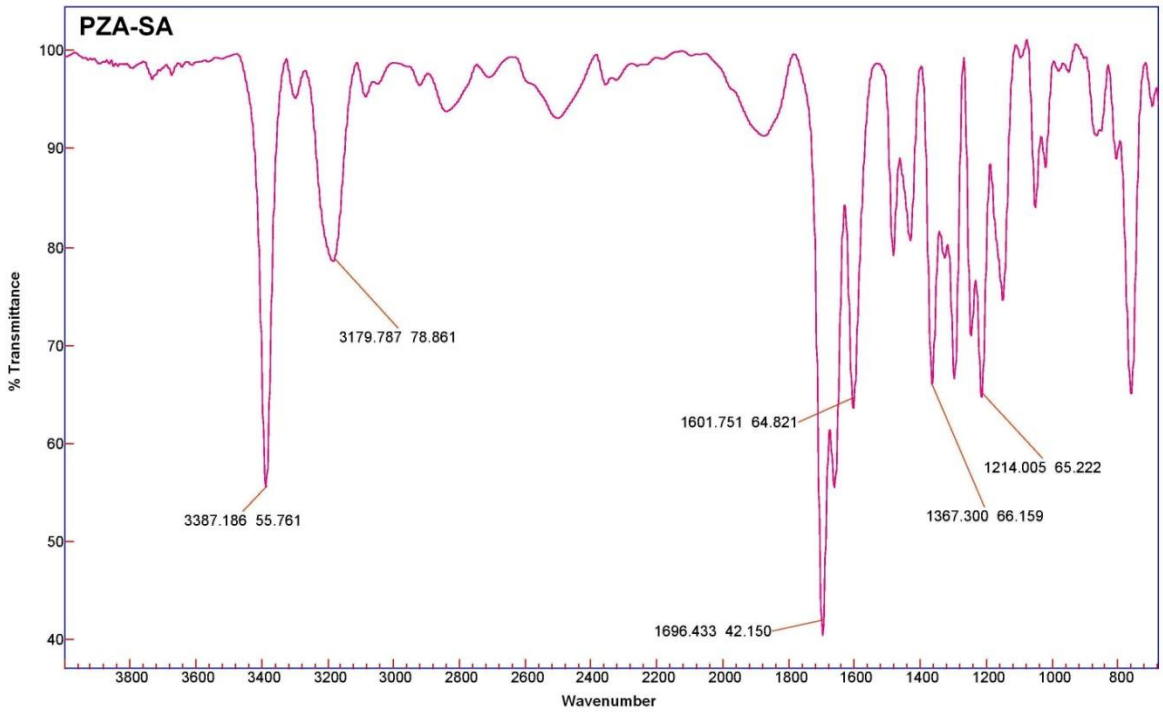


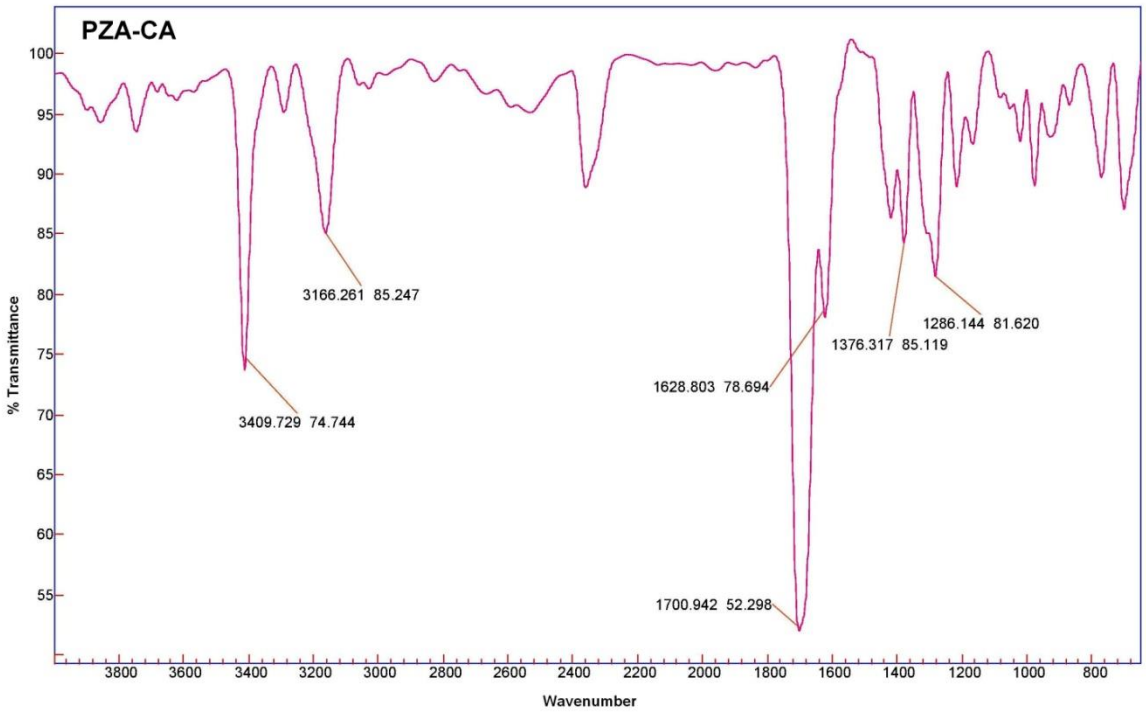
Figure S5. DSC thermograms of PZA-SA eutectic at its eutectic compositions i.e. 1:1 showing lowest melting endotherm coincides with the binary phase diagram.


PZA-BA
% Transmittance
Wavenumber
3166.261 78.288
3414.238 63.761
1606.259 80.201
1430.421 78.876
1376.317 75.982
1705.450 37.545

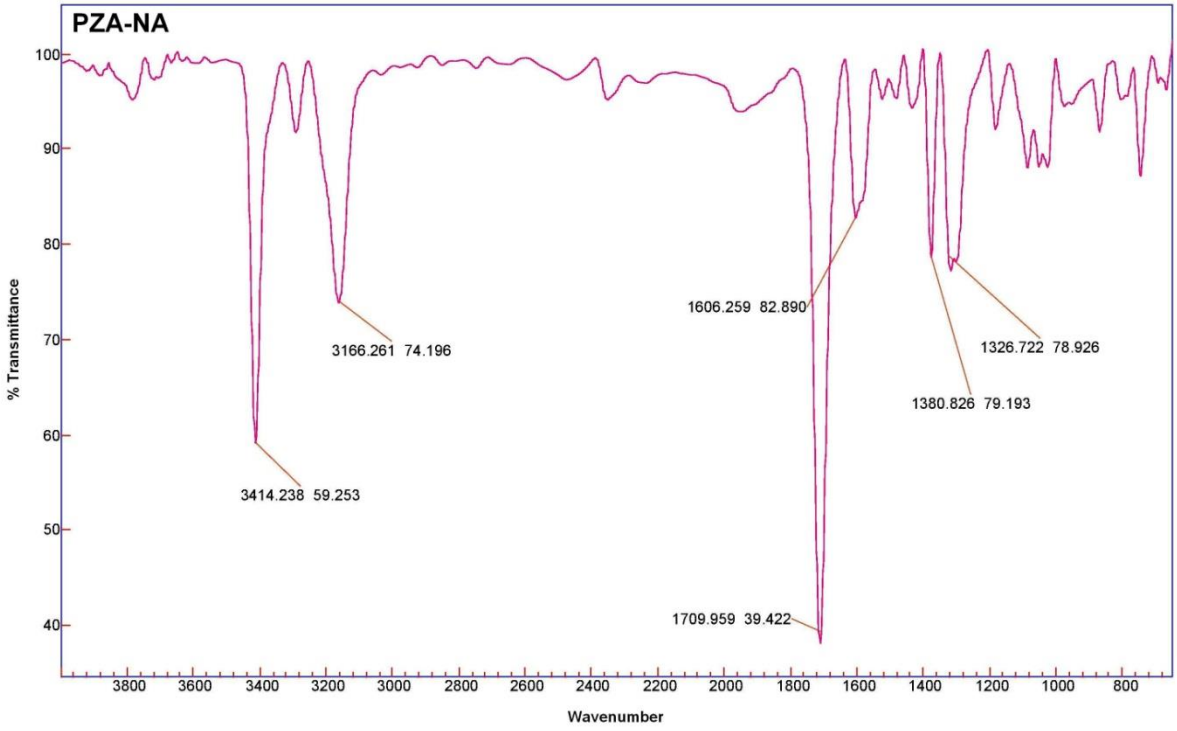
(a)


PZA-SA
% Transmittance
Wavenumber
3179.787 78.861
3387.186 55.761
1601.751 64.821
1214.005 65.222
1367.300 66.159
1696.433 42.150

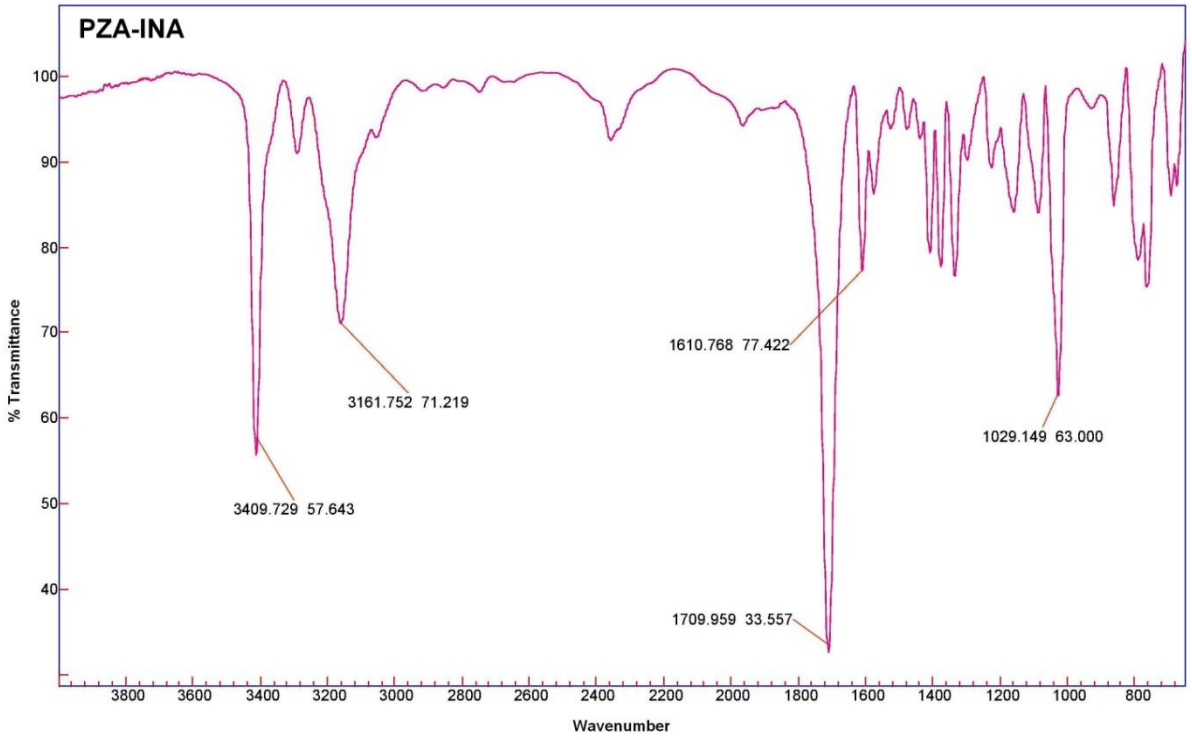
(b)


PZA-CA
% Transmittance
Wavenumber
3166.261 85.247
3409.729 74.744
1628.803 78.694
1376.317 85.119
1286.144 81.620
1700.942 52.298

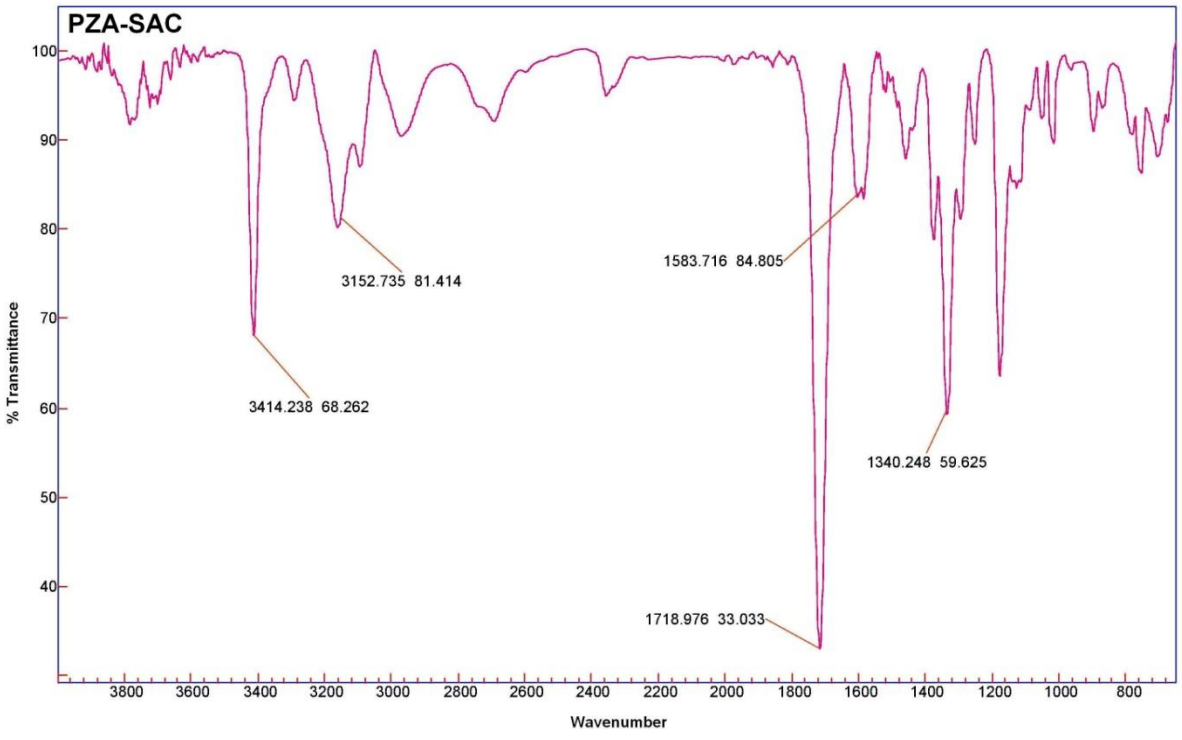
(c)


PZA-NA
% Transmittance
Wavenumber
3166.261 74.196
3414.238 59.253
1606.259 82.890
1326.722 78.926
1380.826 79.193
1709.959 39.422

(d)


PZA-INA
% Transmittance
Wavenumber
3409.729 57.643
3161.752 71.219
1610.768 77.422
1709.959 33.557
1029.149 63.000

(e)


PZA-SAC
% Transmittance
Wavenumber
3414.238 68.262
3152.735 81.414
1583.716 84.805
1718.976 33.033
1340.248 59.625

(f)

Figure S6. FT-IR spectra of the respective eutectic systems (a) PZA–BA, (b) PZA–SA, (c) PZA–CA, (d) PZA–NA, (e) PZA–INA and (f) PZA–SAC.