Electronic Supplementary Material (ESI) for CrystEngComm

Microwave assisted synthesis of caffeine/maleic acid co-crystals: the role of the dielectric and physicochemical properties of the solvent

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Supporting Information

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SI.1 PXRD of solvent free batches:

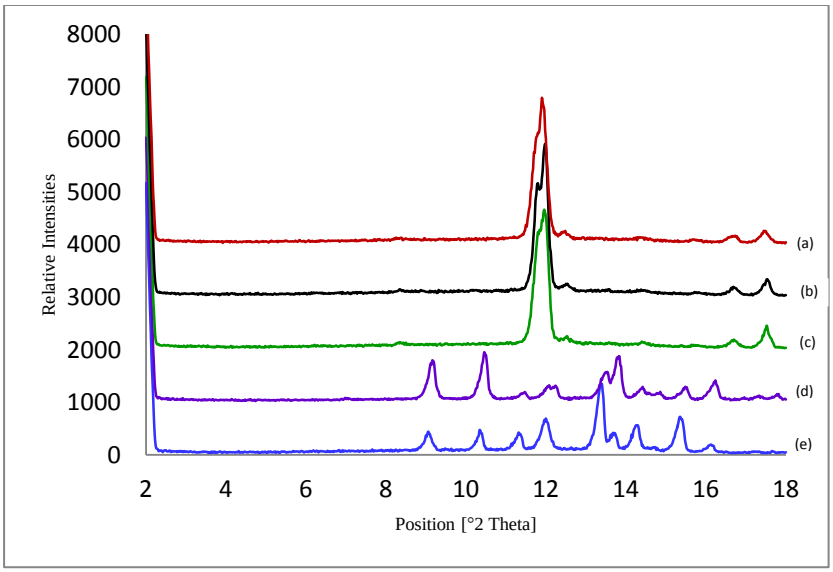


Fig.1 PXRD pattern of solvent free trials processed at (a) 80 °C with 90 sec hold time, (b) 80 °C with 60 sec hold time, (c) 80 °C with 30 sec hold time, (d) 100 °C with 2 min hold time and (e) 100 °C with 5 min hold time.

SI.2 PXRD of solvent mediated batches of 1:1 caf/ma mixture with 2% solvent addition at 80 °C

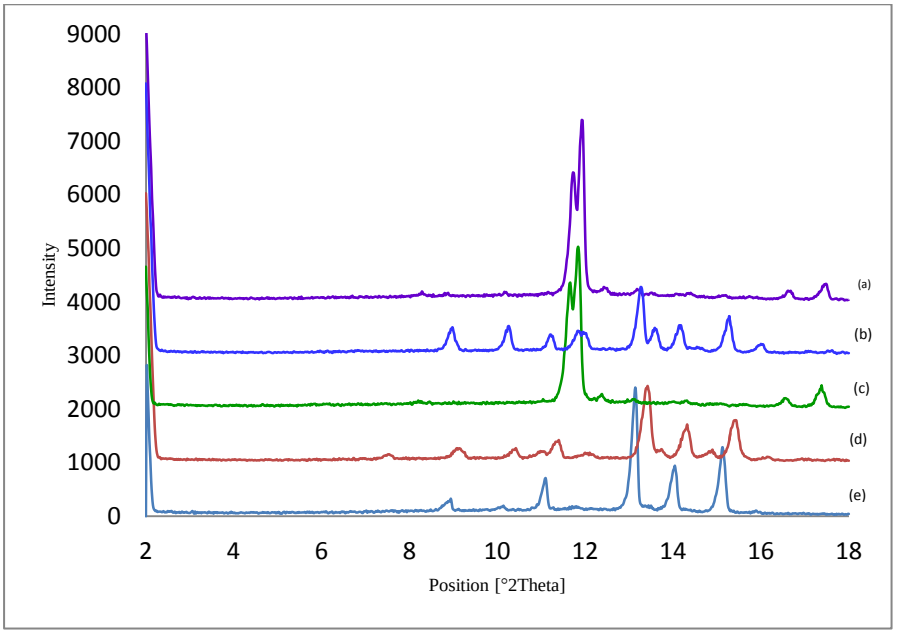


Fig.2 PXRD pattern of solvent mediated batches of 1:1 caf/ma mixture with 2% solvent addition (a) Toluene, (b) Ethyl acetate, (c) Acetone, (d) Methanol and (e) Water.

SI.3 PXRD of solvent mediated batches of 1:1 caf/ma mixture with 4% solvent addition

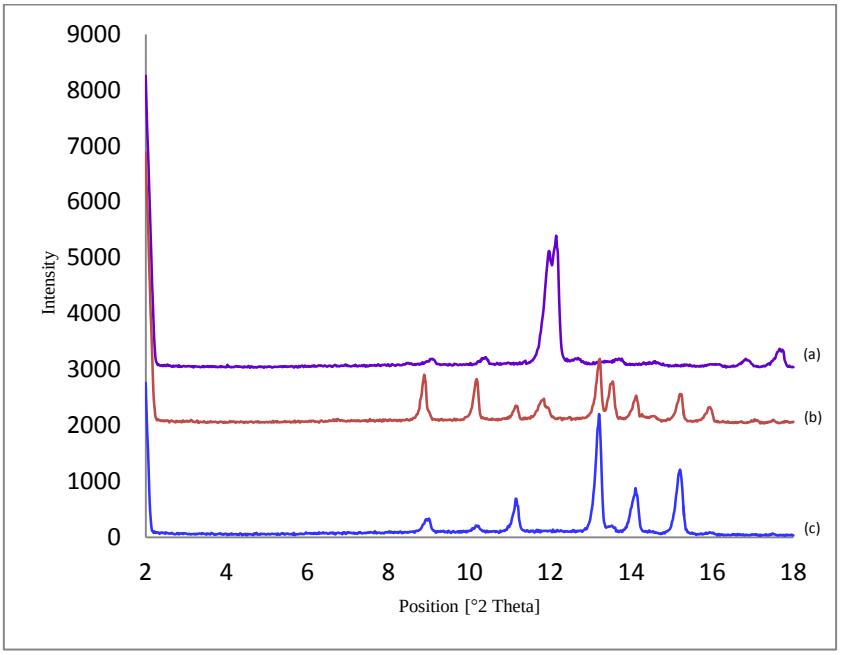


Fig.3 PXRD pattern of PXRD of solvent mediated batches of 1:1 caf/ma mixture with 4% solvent addition (a) Toluene, (b) Ethyl acetate and (c) Water.

SI.4 PXRD of solvent mediated batches of 1:1 caf/ma mixture with 10% solvent addition

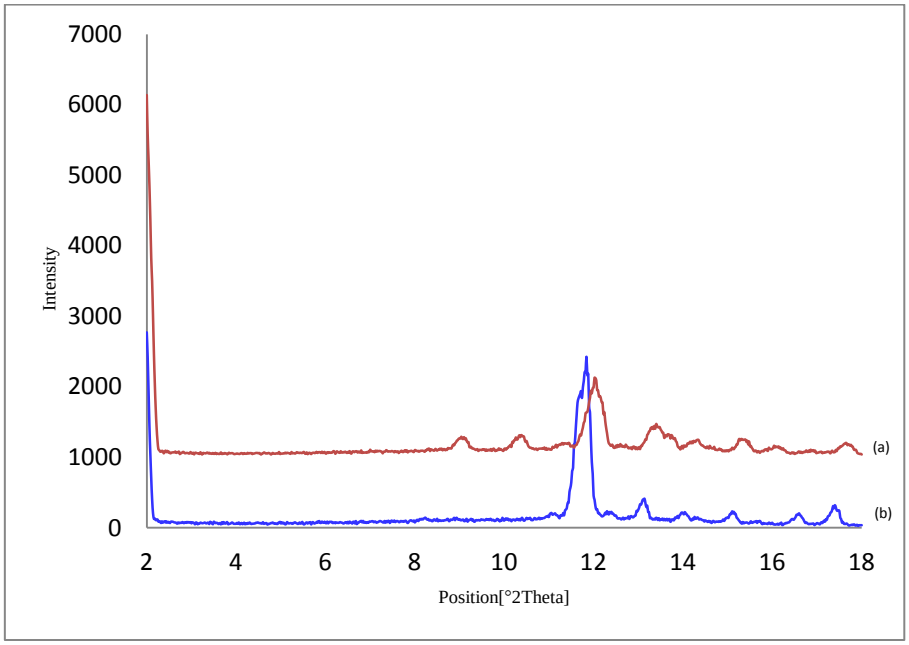


Fig.4 PXRD pattern of solvent mediated batches of 1:1 caf/ma mixture with 10% solvent addition (a) Toluene and (b) Acetone.

SI.5 PXRD of solvent mediated batches of 2:1 caf/ma mixture with 2% solvent addition at 80 °C

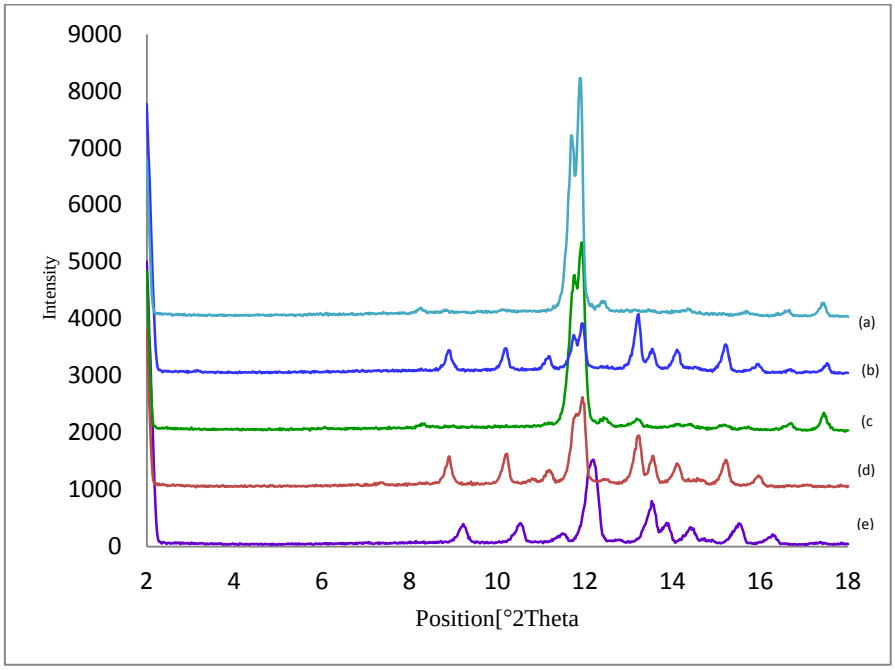


Fig.5 PXRD pattern of solvent mediated batches of 2:1 caf/ma mixture with 2% solvent addition (a) Toluene, (b) Ethyl acetate, (c) Acetone, (d) Methanol and (e) Water.

SI.6 PXRD of solvent mediated batches of 2:1 caf/ma mixture with 4% solvent addition

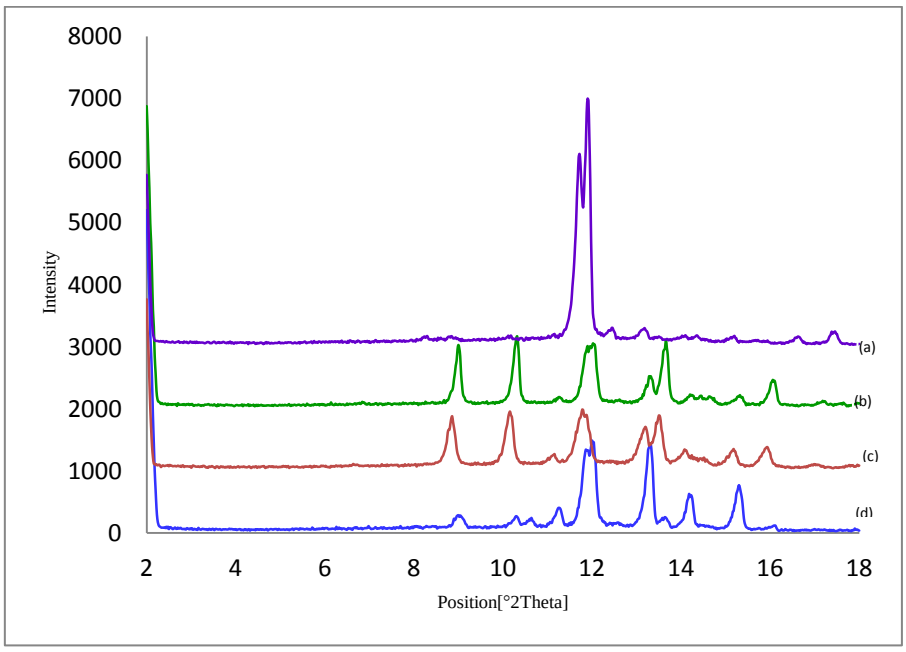


Fig.6 PXRD pattern of solvent mediated batches of 2:1 caf/ma mixture with 4% solvent addition (a) Toluene, (b) Ethyl acetate, (c) Acetone and (d) Water.

SI.7 PXRD of solvent mediated batches of 2:1 caf/ma mixture with 10% addition of methanol at 80 °C

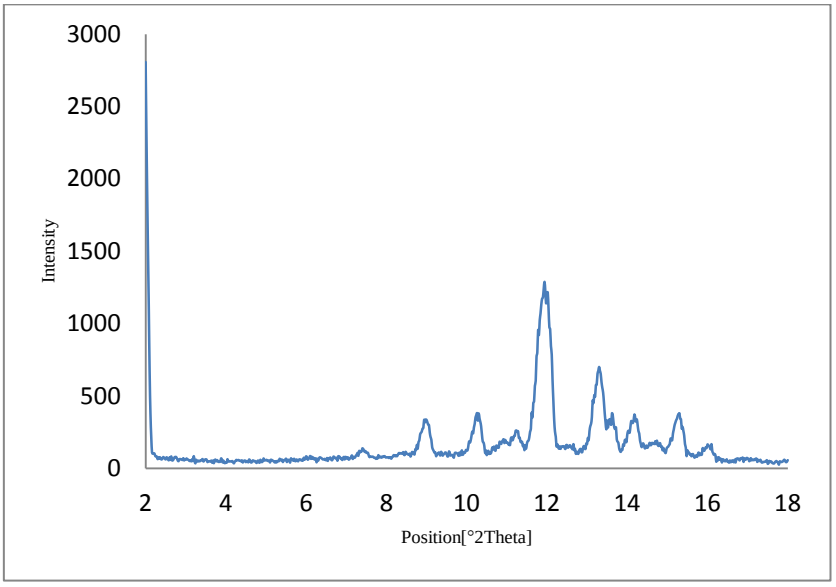


Fig.7 PXRD pattern of caf/ma 2:1 physical mixture after addition of 10% Methanol and heated to 80 °C under microwave.

SI.8 PXRD pattern of untreated samples and solution crystallisation

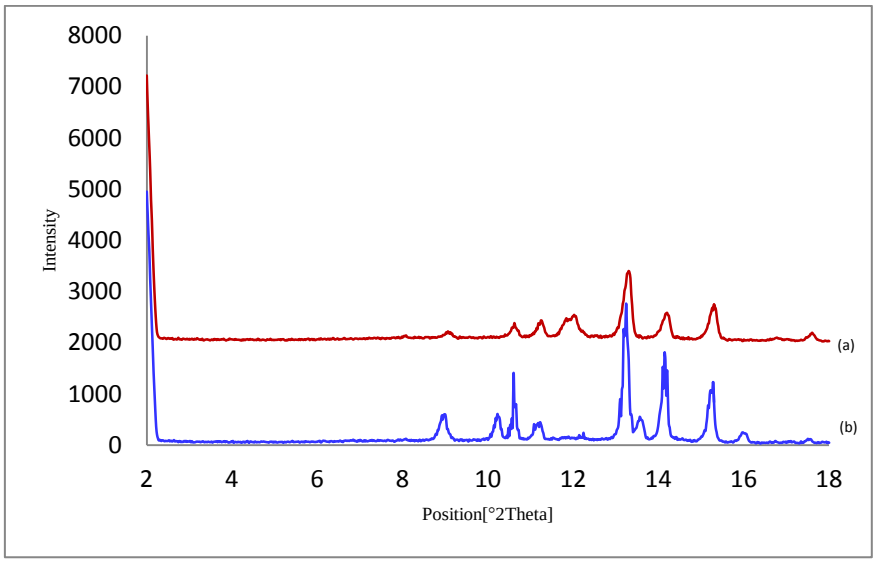


Fig.8 PXRD pattern of (a) **caf**/**ma** 1:1 mixture with 10% of water without microwave treatment, (b) crystallisation of 1:1 **caf**/**ma** mixture from water, solution crystallisation.

SI.9 PXRD pattern of caffeine and maleic acid

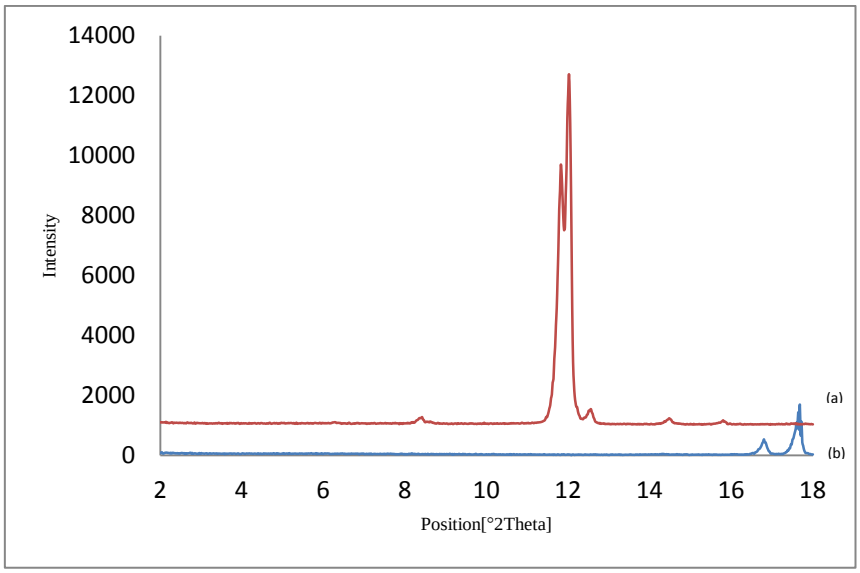


Fig.9 PXRD pattern of caffeine (a) and (b) maleic acid

SI.10 Microwave power uptake profiles for pure solvent

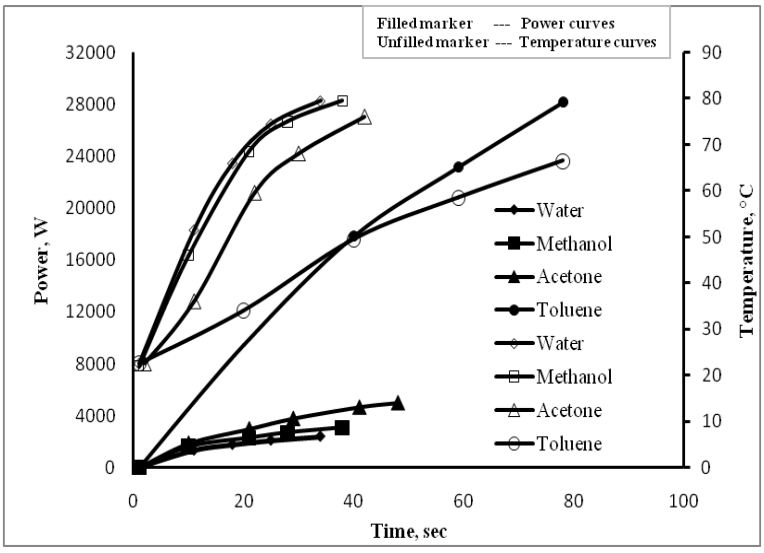


Fig.10 Temperature and power uptake curves for water, methanol, acetone and toluene.

SI.11 Highest occupied molecular orbital (HOMO) and Lowest unoccupied molecular orbital (LUMO) with Dipole moment of caffeine and maleic acid

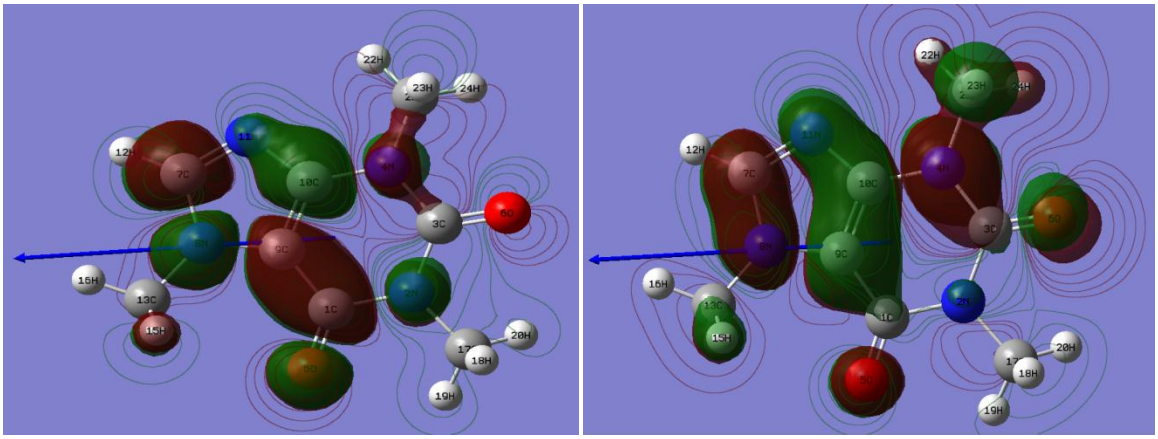
Caffeine

T.E. = -0.07863776 au

RMS gradient Norm = 0.00000459au

Dipole= 3.9131 Debye in x=-3.8968, y= 0.1824, z= 0.3067

Positive = red , Negative =green, iso value=0.0 2



Maleic acid

T.E. = -0.25871448 au

RMS gradient Norm = 0.00000567au

Dipole= 4.5825 Debye in x=-3.3878, y= -3.0858, z= 0.0020

Positive = red , Negative =green, iso value=0.0 2