

## SUPPORTING INFORMATION FOR:

### Jet dispensing as a high throughput method for rapid screening and manufacturing of cocrystals

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#### Experimental

*Materials:* Indomethacin saccharin and all the solvents (ethanol, Acetone, Methanol; HPLC grade) were purchased from Sigma-Aldrich (UK).

*Jet dispensing:* The jet dispensing was performed with a Nordson Asymtek (Netherlands) dispense mate equipped with a DJ 9000 dispenser. The size of the nozzle and the seat used was 100  $\mu\text{m}$  and 300  $\mu\text{m}$ , respectively. The needle size was 2.4 mm and the fluid pressure 10 bar. An array of 10x10 droplets were deposited on Silicon substrate suitable for XRPD analysis.

*Scanning Electron Microscopy (SEM):* In order to analyse the crystals' topography, a SEM (Hitachi SU8030, Japan) at 10 kV accelerating voltage was used. Samples were placed on double sided carbon tape sticks on an aluminium stub and coated with a thin layer of chromium in an argon atmosphere at room temperature by using an EMITECH K575X sputter coater (Quorum Technologies, Sussex, UK).

*X-ray powder diffraction (XRPD):* XRPD was used to determine the solid state of bulk materials, physical mixtures and extrudates using a Bruker D8 Advance (Germany) in theta-theta mode. For the study purposes a Cu anode at 40 kV and 40 Ma, parallel beam Goebel mirror, 0.2 mm exit slit, LynxEye Position Sensitive Detector with 3° opening (LynxIris at 6.5 mm) and sample rotation at 15 rpm were used. Each sample was scanned from 2 to 40° 2 $\theta$  with a step size of 0.02° 2 $\theta$  and a counting time of 1 sec per step. Quantitative XRD was calculated using Rietveld refinement and were performed with TOPAS version 4.2 using a fundamental parameters approach with full axial model. Refined parameters for each phase included lattice parameters and crystallite size, values for atomic coordinates and site occupancies were fixed.

*Fourier transform infrared (FT-IR) spectroscopy:* IR spectra were recorded on a Perkin - Elmer Spectrum RX I FT-IR spectrometer. Samples were prepared in KBr disks prepared with a hydrostatic press. The scanning range was 450–4000  $\text{cm}^{-1}$  at 1  $\text{cm}^{-1}$  resolution.

*Differential scanning calorimetry (DSC):* DSC studies were performed using a Q2000 (TA Instruments) calorimeter under a nitrogen atmosphere at a flow of 100 mL  $\text{min}^{-1}$ , using hermetically sealed with a pin hole in the lid.. Samples were prepared in sealed Tzero aluminium pans (2–5 mg) with a pierced lid in triplicates. The samples were heated at 10  $^{\circ}\text{C}/\text{min}$  in a temperature range between 25 and 250  $^{\circ}\text{C}$ .

*In-vitro dissolution studies:* In-vitro dissolution study carried out by using a Varian 705 DS dissolution paddle apparatus (Varian Inc., Lake Forest, CA, USA) at 100 rpm and  $37.0 \pm 0.5$   $^{\circ}\text{C}$ . The dissolution medium was a 750 ml phosphate buffer at 7.2. At predetermined time intervals (e.g. ...), samples were withdrawn for HPLC assay. All dissolution studies were performed in triplicate.

*Drug content analysis:* HPLC analysis was carried out using an AGILENT 1200 series HPLC (USA) instrument equipped with an autosampler. The mobile phase was prepared with a 70% methanol, 30 % water and 0.2 % acetic acid. A Zorbax Eclipse C8 ( $4.6 \times 150 \text{ mm} \times 5 \mu\text{m}$ ) column from Agilent, USA was used with a 1 ml  $\text{minute}^{-1}$  flow rate at a 260 nm wavelength. The calibration curve was constructed by varying the standard solution concentration from 10–50  $\mu\text{g ml}^{-1}$ .

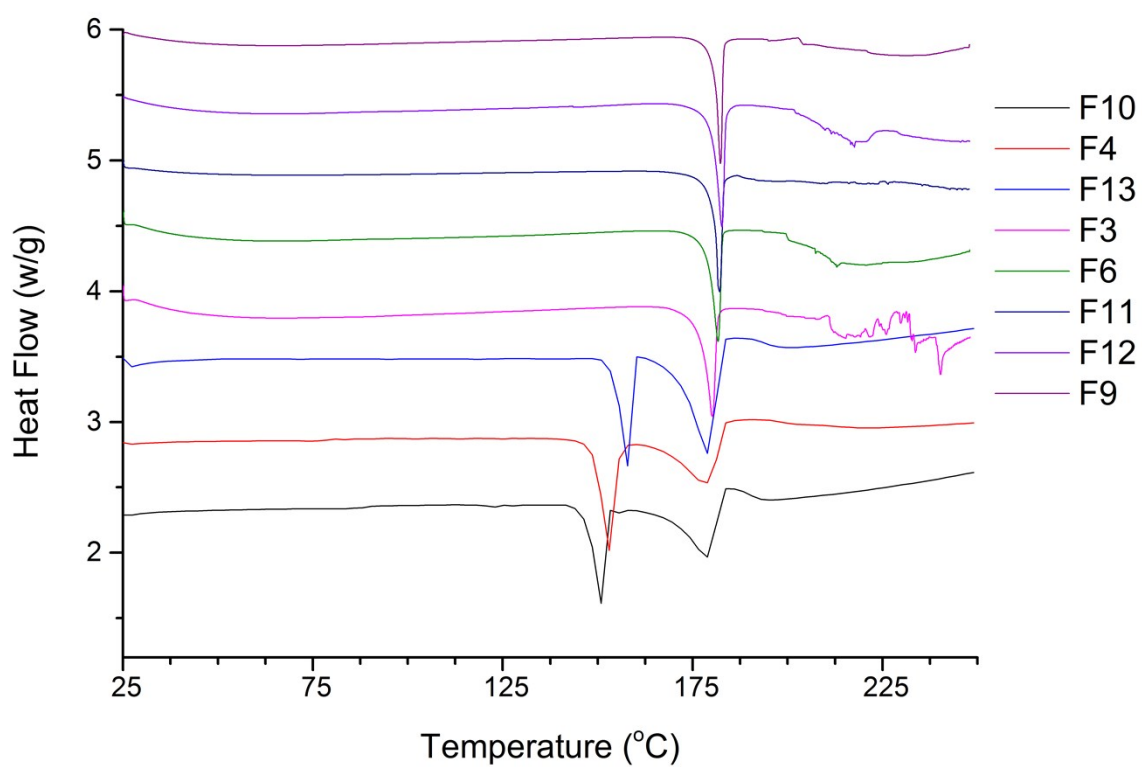


Figure S1: DSC thermographs of cocrystals. The graphs shows that all the experiments produced cocrystals. However, the first peak of F10, F4 and F13 indicates a part of IND that did not form co-crystal. Whereas the second endothermic peak in the rest experiments are SCH which did not form cocrystal.

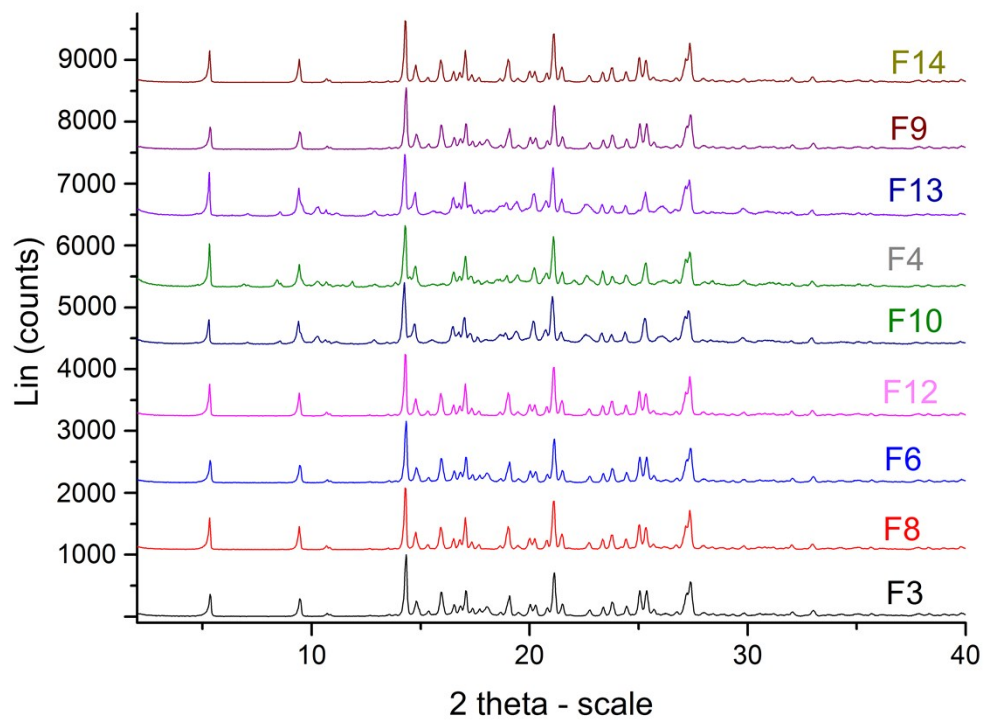


Figure S2: XRD diffractograms of cocrystals. All the XRD graphs contain the characteristic peaks of cocrystal. However, TOPAS analysis showed that F4, F10, F13 contains peak pattern coming from IND whereas the rest contains SCH.

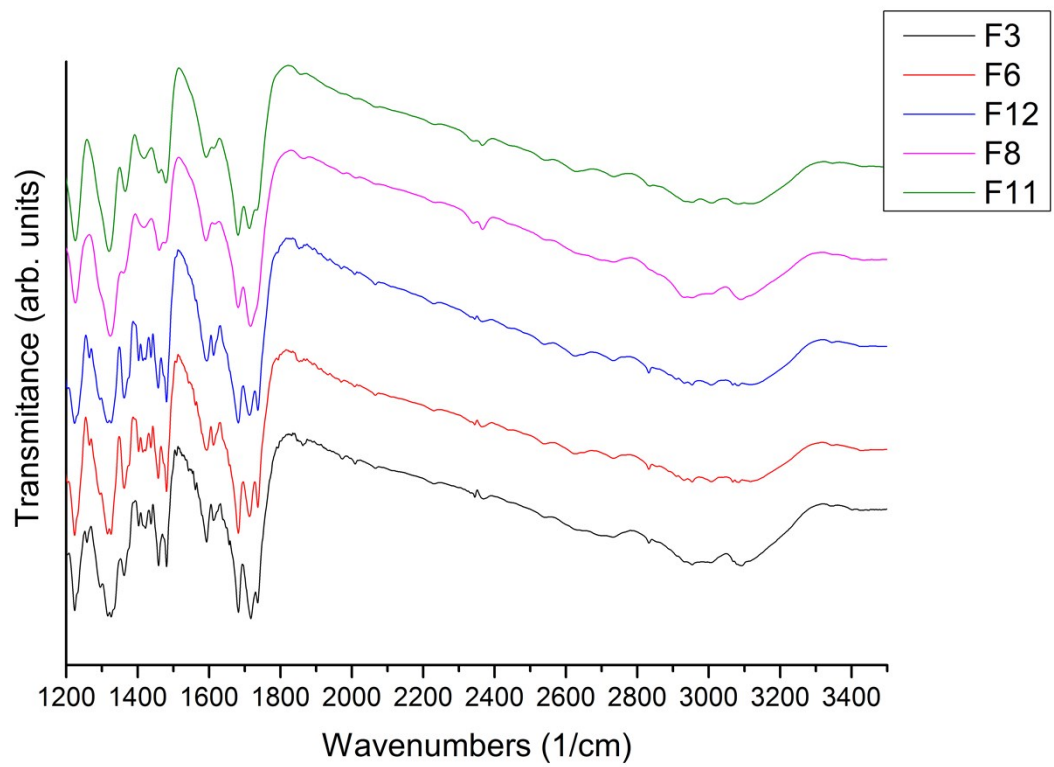


Figure S3: FT-IR spectra of cocrystals. The FT-IR showed the same results similar to the one represented in manuscript which confirm the formation of cocrystal.