

## Electronic supplementary information

### **Solvent penetration mediated phase transformation: a method for well - defined shape of aggregated particles**

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### **Materials and instruments**

Raw material of sulfadiazine was from PKU Health Care Co. Ltd., China. N-methyl pyrrolidone (NMP) solvent was purchased from Tianjin Kewei Chemical Co. Ltd., China. Deionized water was produced using a Millipore system. The morphology of samples was determined using analytical scanning electron microscope (TM3000, Hitachi, Japan). The phase form was analysed by a X-ray powder diffractometer (model D/max-2500, Rigaku).

### **Preparation of different shapes of NMP solvate particles.**

#### 1) Preparation of rod-like shape of NMP solvate particles

8 g sulfadiazine powder was added to 60 g NMP solvent into a sample bottle and was heated to 60 °C to obtain clear solution. The solution was placed directly at room temperature environment ( $18 \pm 1$  °C) to lead to a high degree supersaturation. Nucleation was occurred immediately. After 1 h, the crystallized residue was filtered. The obtained particles are rod-like.

#### 2) Preparation of rhombic shape of NMP solvate particles

8 g sulfadiazine powder was added to 60 g NMP solvent into a crystallizer

connected to a thermostat bath and was heated to 60 °C to obtain clear solution. A propeller-type agitator was used to stir the crystallization mixture. The supersaturation was obtained by linear cooling down the solution to room temperature. To reach the final temperature, the system took 3 h. The crystallized residue was filtered. The obtained particles are rhombic.

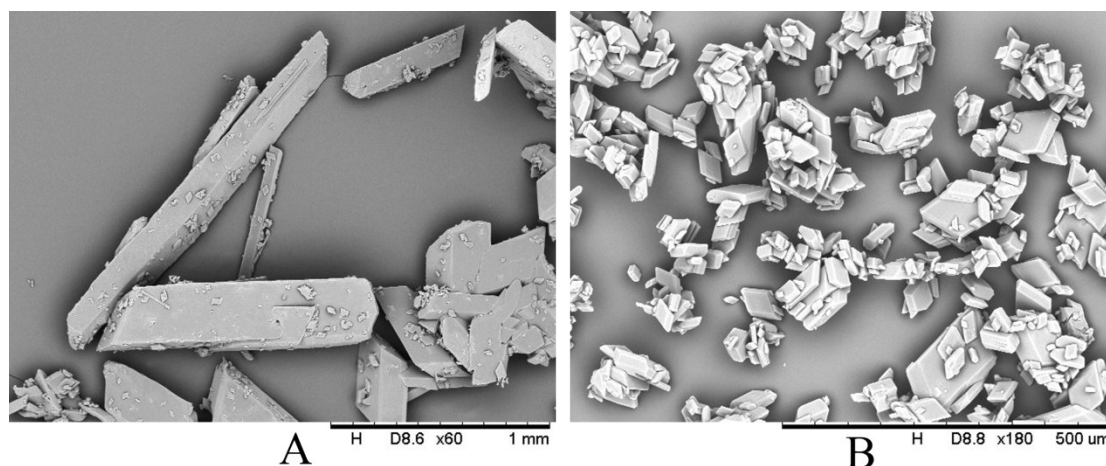


Figure S1 (A) the rod-like shape of NMP solvate particles prepared by rapid cooling crystallization, (B) the rhombic shape of NMP solvate particles prepared by slow cooling crystallization.

### **Preparation of sulfadiazine aggregates by solvent mediated phase transformation**

3g prepared NMP solvate powder was added to 40 mL of water. The suspension was stirred at 100 rpm at room temperature. The solution (~ 10 mL) was filtered respectively at 1 min, 2 min and 60 min after the powder was added to water. The solid phase obtained was confirmed using PXRD and SEM. It can be confirmed that the NMP solvate powder has transformed into sulfadiazine particles completely in 1 minute.

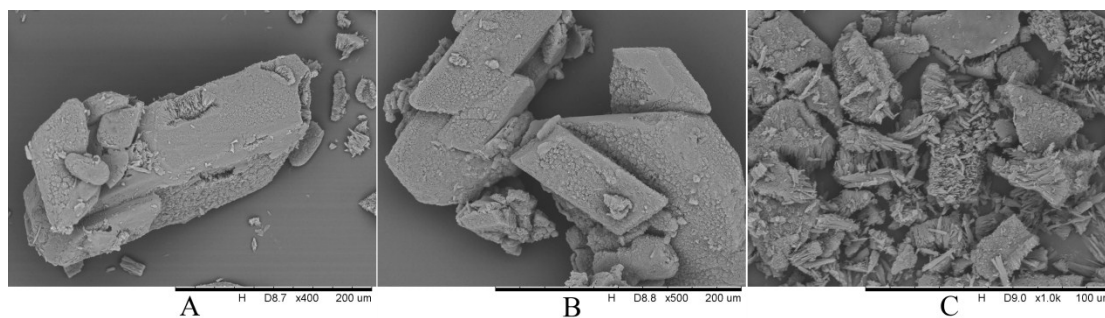


Figure S2 (A) the obtained particles after 1 min, (B) the obtained particles after 2 min (C) the obtained particles after 60 min

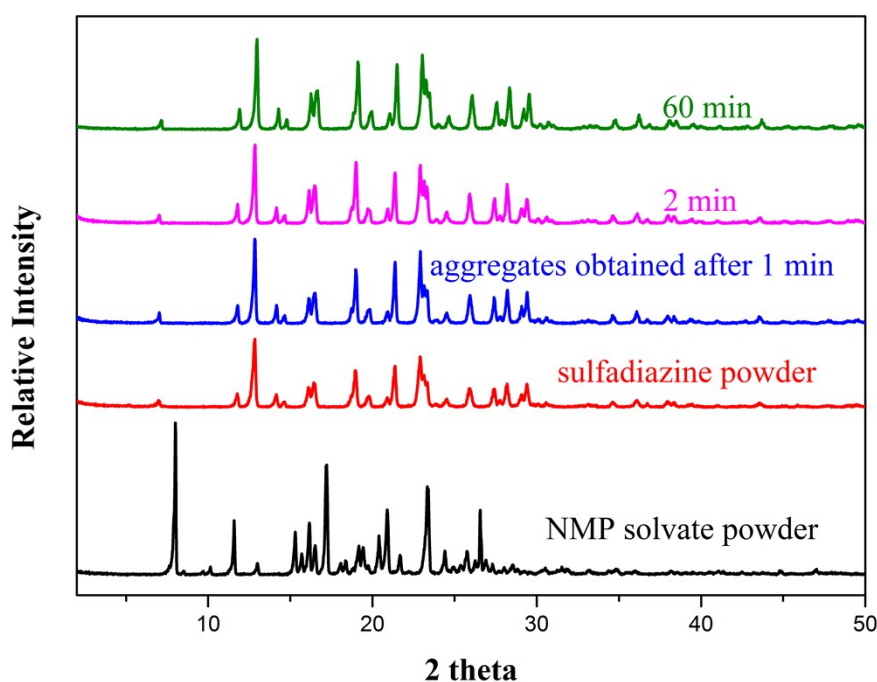


Figure S3 the PXRD spectra of sulfadiazine powder, NMP solvate powder and aggregates obtained from NMP solvate particles suspended in water for 1 min, 2 min and 60 min.

### The effect of solvent composition on the transformation rate

The mixed solvent NMP/water (1:2, 1:1, 2:1) was chosen to research the impact of solvent on the transformation rate.

The experimental results show that the impact of the content of NMP in solvent on the phase transformation rate is very small when the content of NMP is below 50%, the whole phase transformation can be finished in one minute. When the content of NMP/water is 2:1, the dissolution effect of solvent on NMP solvate cannot be ignored.

The transformation rate was decreased obviously and the whole phase transformation process was finished in 20 minutes.