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*Electronic Supplementary Information for*

# Effects of various parameters on solution-mediated phase transformation of calcium D-gluconate: An approach to obtain pure metastable monohydrate

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Table S1. Calcium D-gluconate SMPT experimental parameters in 100 g water

| | Temperature/K | Solid loading/g | Stirring speed/rpm | Particle size /μm |
|---|---|---|---|---|
| 1 | 353.15 | 5.6 | 200 | 3.36 |
| 2 | 348.15 | 5.6 | 200 | 3.36 |
| 3 | 338.15 | 5.6 | 200 | 3.36 |
| 4 | 348.15 | 6.6 | 200 | 3.36 |
| 5 | 348.15 | 4.3 | 200 | 3.36 |
| 6 | 348.15 | 4.3 | 400 | 3.36 |
| 7 | 348.15 | 4.3 | 600 | 3.36 |
| 8 | 353.15 | 5.6 | 200 | 2.21 |
| 9 | 353.15 | 5.6 | 200 | 1.77 |

Table S2. Parameters and Coefficients of Determination of the Modified Apelblat Equation for the Solubility of calcium gluconate monohydrate and Form I

| Parameters | *A* | *B* | *C* | $R^2$ |
|---|---|---|---|---|
| monohydrate | -129.35 | 2973.56 | 19.80 | 0.998 |
| Form I | -160.77 | 5111.59 | 24.04 | 0.998 |

Table S3. Solubility data of calcium D-gluconate in water (mole fraction)

| Temperature/K | monohydrate | Temperature/K | Form I |
|---|---|---|---|
| 283.15 | 0.00092 | 278.15 | 0.00092 |
| 288.15 | 0.00102 | 288.15 | 0.00104 |
| 290.15 | 0.00105 | 290.15 | 0.00107 |
| 293.15 | 0.00116 | 293.15 | 0.00109 |
| 303.15 | 0.00160 | 303.15 | 0.00151 |
| 308.15 | 0.00194 | 313.15 | 0.00188 |
| 313.15 | 0.00231 | 323.15 | 0.00240 |
| 323.15 | 0.00312 | 333.15 | 0.00309 |
| 333.15 | 0.00428 | 338.15 | 0.00359 |
| 343.15 | 0.00630 | 343.15 | 0.00423 |
| 353.15 | 0.00834 | 353.15 | 0.00530 |

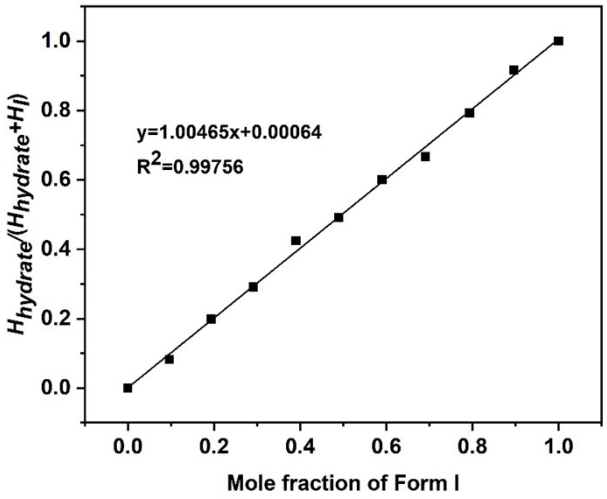


Fig. S1 Calibration model of Raman spectra of calcium D-gluconate fraction.

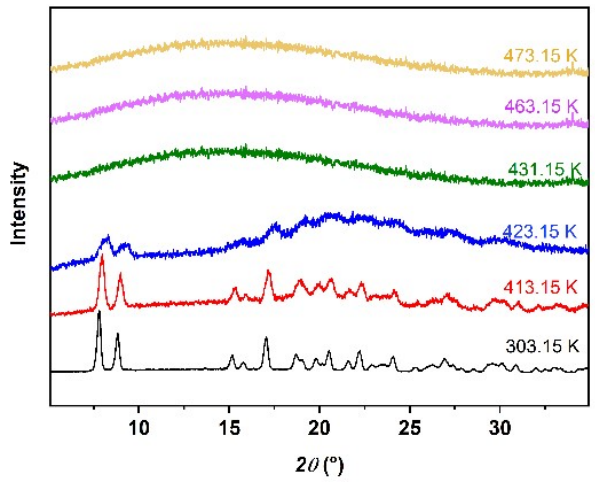


Fig.S2 VT-XRD patterns of calcium gluconate monohydrate at different temperature.

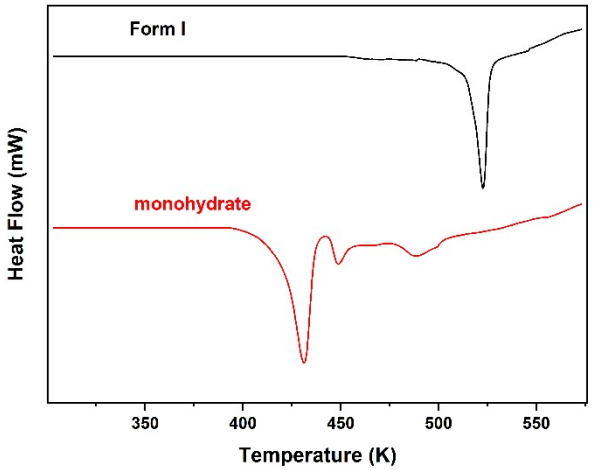


Fig.S3 DSC thermograms of calcium gluconate Form I and monohydrate.

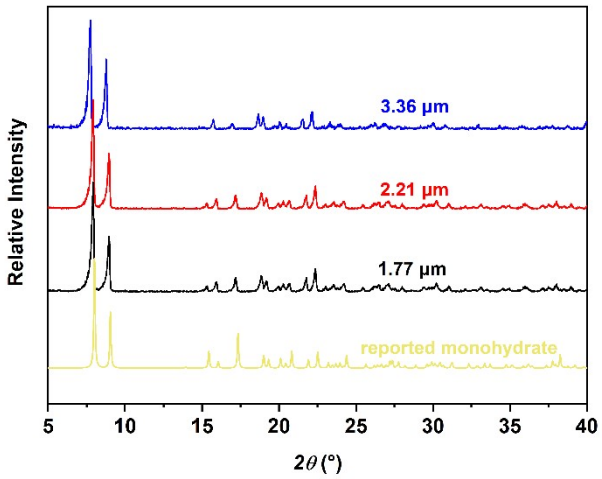


Fig.S4 PXRD patterns of calcium gluconate monohydrate with different particle sizes after grinding.

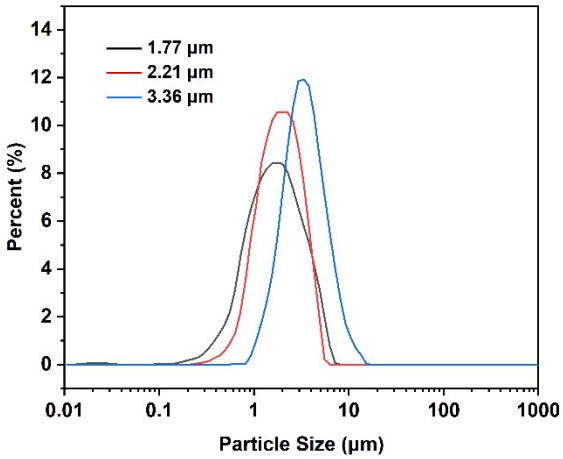


Fig.S5 The particle size distributions of calcium gluconate monohydrate with different particle sizes after grinding.