Electronic Supplementary Information for

Explanation and Prediction for the Selective Crystallization of Boscalid by Mid-Frequency Raman Difference Spectra Analysis

Yingjie Fan,[a,b] Chengfeng Liang, [b] Yanping Li, [b] Wangchuan Xiao, [b] Yu Niu, [b] Hongjun Jin, [a] Rongrong Xue, *[b] and Fenghua Chen *[b]

[a] College of Environmental and Resource Sciences, Fujian Normal University, Fuzhou 350007, Fujian, China.

[b] School of Resources and Chemical Engineering, Sanming University, Sanming 365004, Fujian, China.

Corresponding Authors
**(R. X.) E-mail: rongrongxue@fjsmu.edu.cn.*
**(F. C.) E-mail: fenghuachen@fjsmu.edu.cn.*

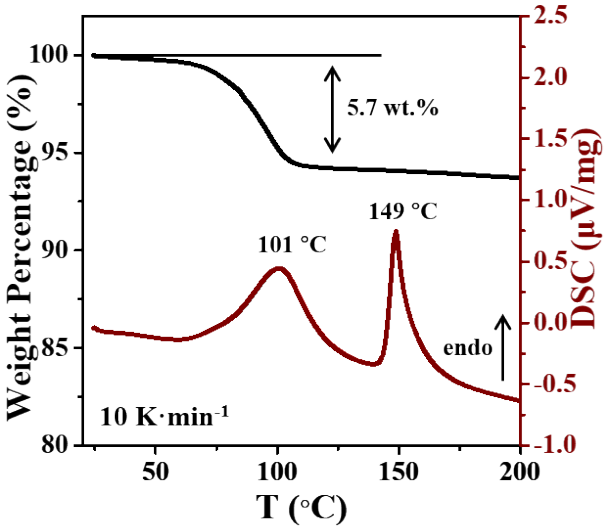

Figure S1. Thermogravimetry-differential scanning calorimetry analysis (TGA-DSC) curve of BOS monohydrate.

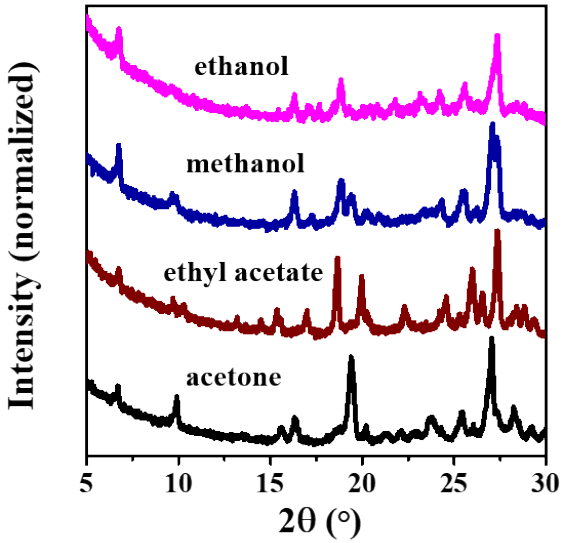

Figure S2. PXRD patterns of BOS monohydrate prepared by anti-solvent method. 1 ml BOS saturated acetone/ethyl acetate/methanol/ethanol solution and 100 ml deionized water were mixed quickly and stirred overnight.

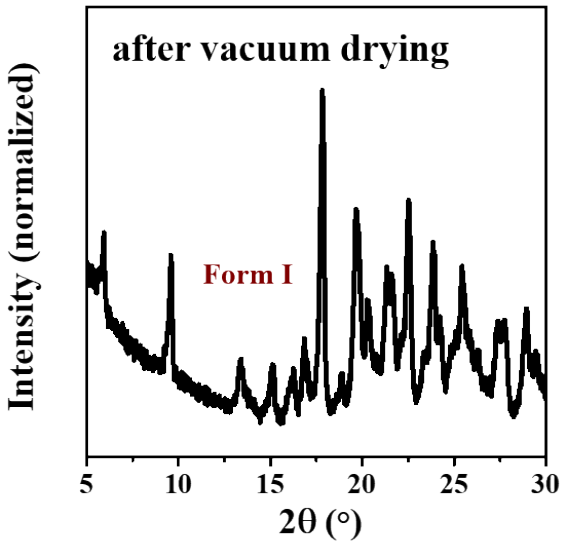

Figure S3. PXRD pattern of BOS monohydrate after vacuum drying overnight.

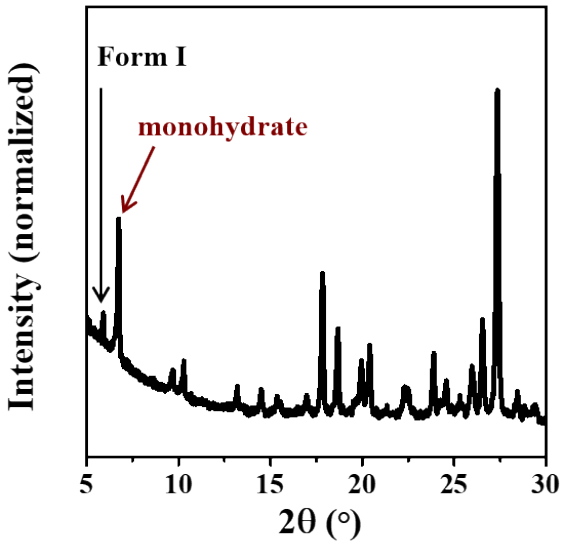

Figure S4. PXRD pattern of the product prepared by evaporation of 50 µl BOS saturated acetone solution at room temperature with low ambient humidity.

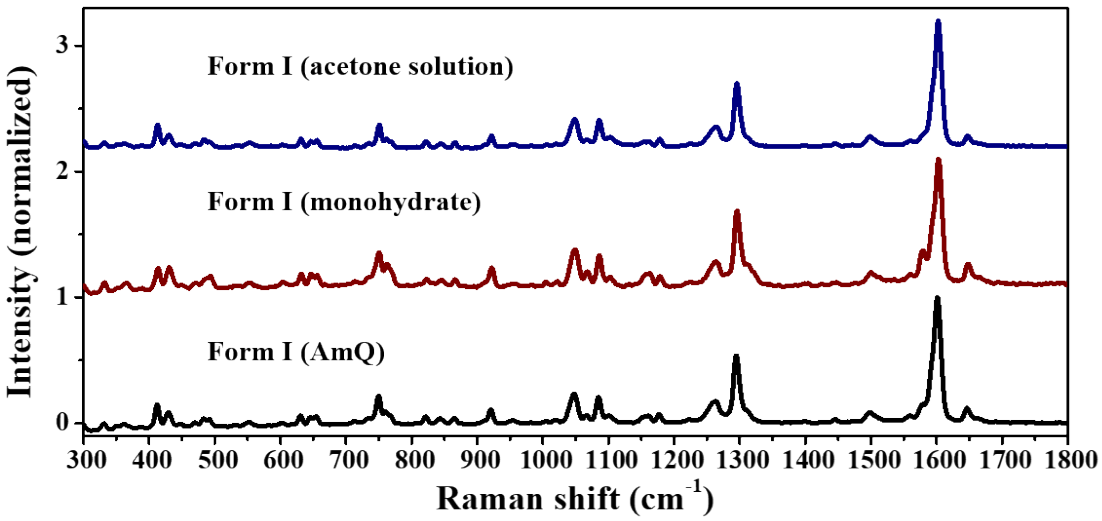

Figure S5. The MFRS of boscalid Form I prepared by different methods in this work. Form I prepared by heating AmQ at 100 °C for 10 min is referred as Form I (AmQ), Form I prepared by heating monohydrate at 100 °C for 10 min is referred as Form I (monohydrate), and Form I prepared by solvent evaporation of 50 µl BOS acetone solution at 60 °C is referred as Form I (acetone solution) here.

Table S1. Summary of the a.d. and s.d. of all the data in the MFRDS with baseline deduction of BOS Form I prepared by the three different methods.

MFRDS	a.d.×10^3	s.d.×10^3
self-Form I (AmQ)	7.8 (2.2)	15 (6)
self-Form I (monohydrate)	4.7 (1.7)	5.9 (2.0)
self-Form I (acetone solution)	9.4 (3.4)	14 (6)
Form I (AmQ) with Form I (monohydrate)	11.5 (2.9)	18 (5)
Form I (AmQ) with Form I (acetone solution)	9.8 (1.6)	15 (4)

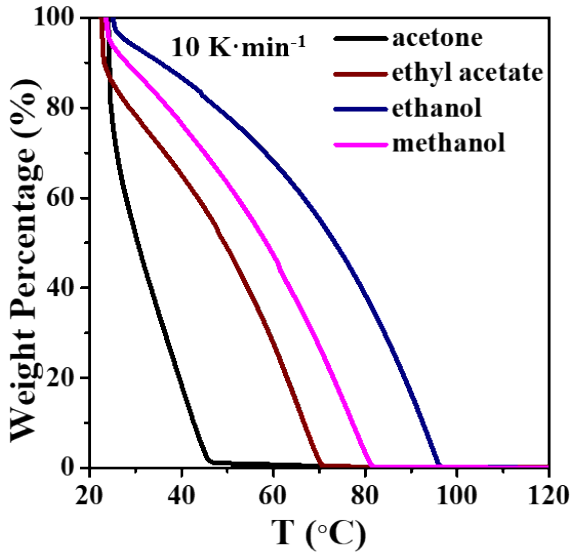

Figure S6. Thermogravimetry curves of 50 μl BOS acetone/ethyl acetate/ethanol/methanol solutions. The residual of BOS solids was set to 0%.

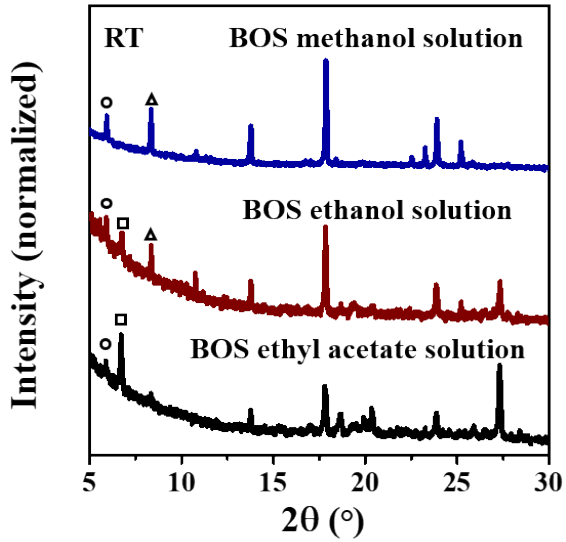

Figure S7. PXRD patterns of the evaporation products of 50 μl BOS saturated ethyl acetate/ethanol/methanol solution at room temperature in a day without rain (○ Form I, △ Form II, □ monohydrate).

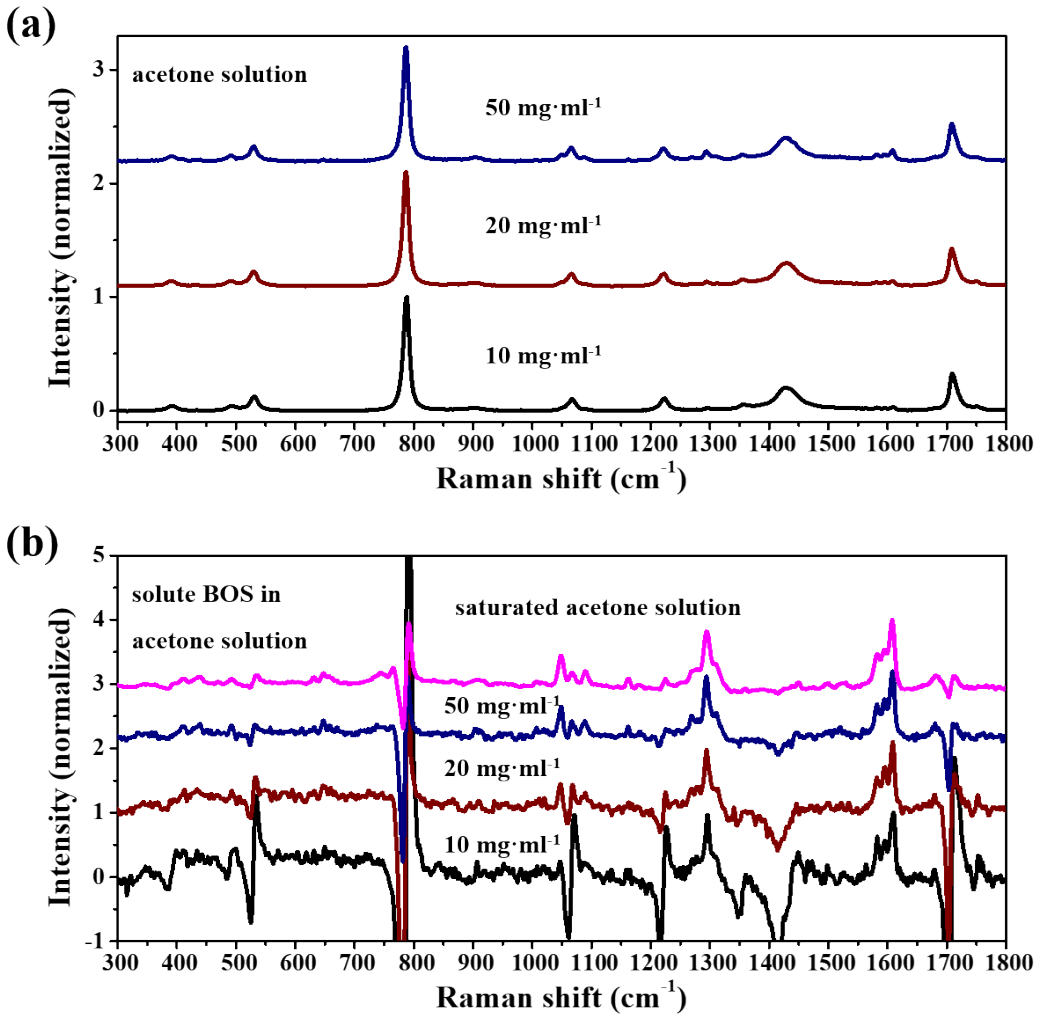

Figure S8. (a) MFRS of BOS acetone solutions with different concentrations, (b) MFRS of solute BOS in acetone solutions with different concentrations.