

**(Supporting Information)**

**In situ monitoring of anti-solvent co-crystallization by combining NIR and  
Raman spectroscopies**

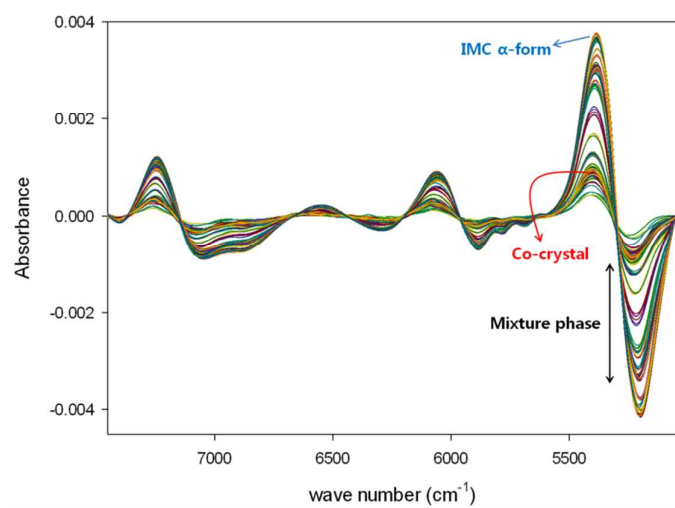
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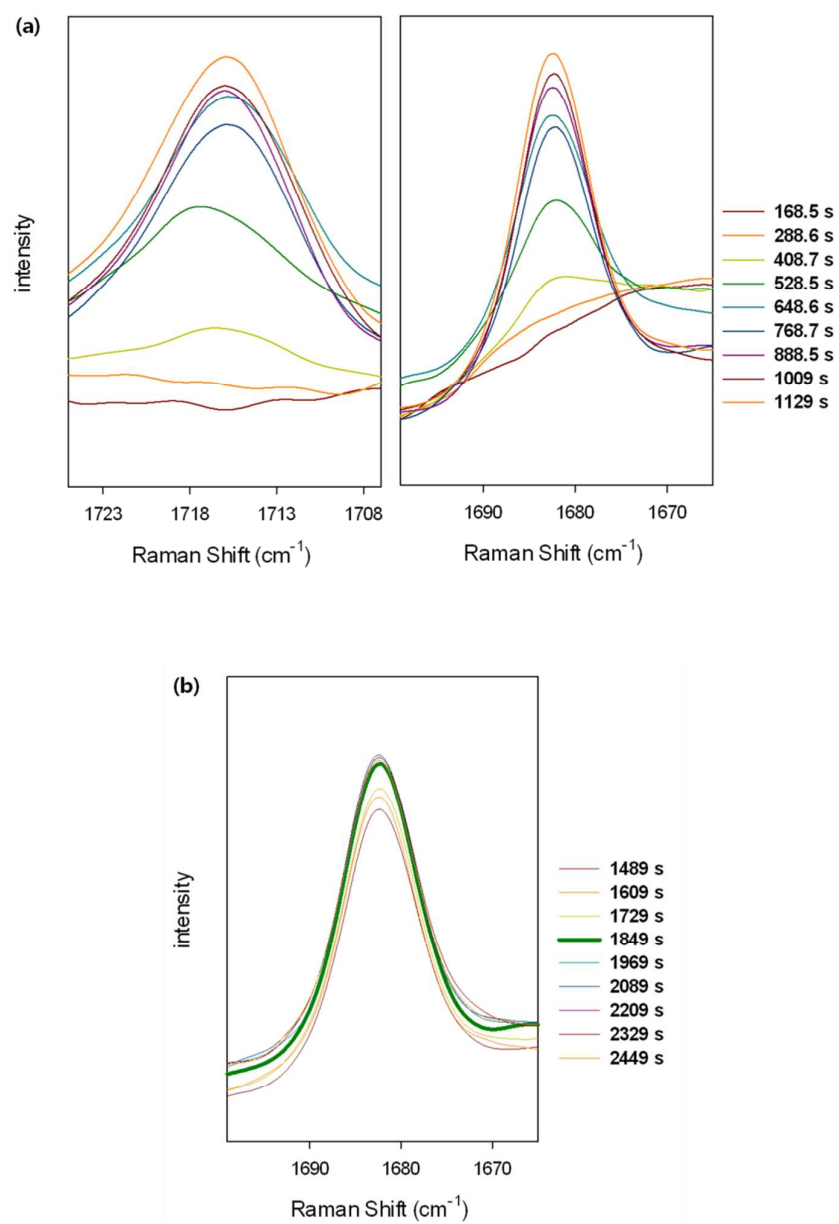
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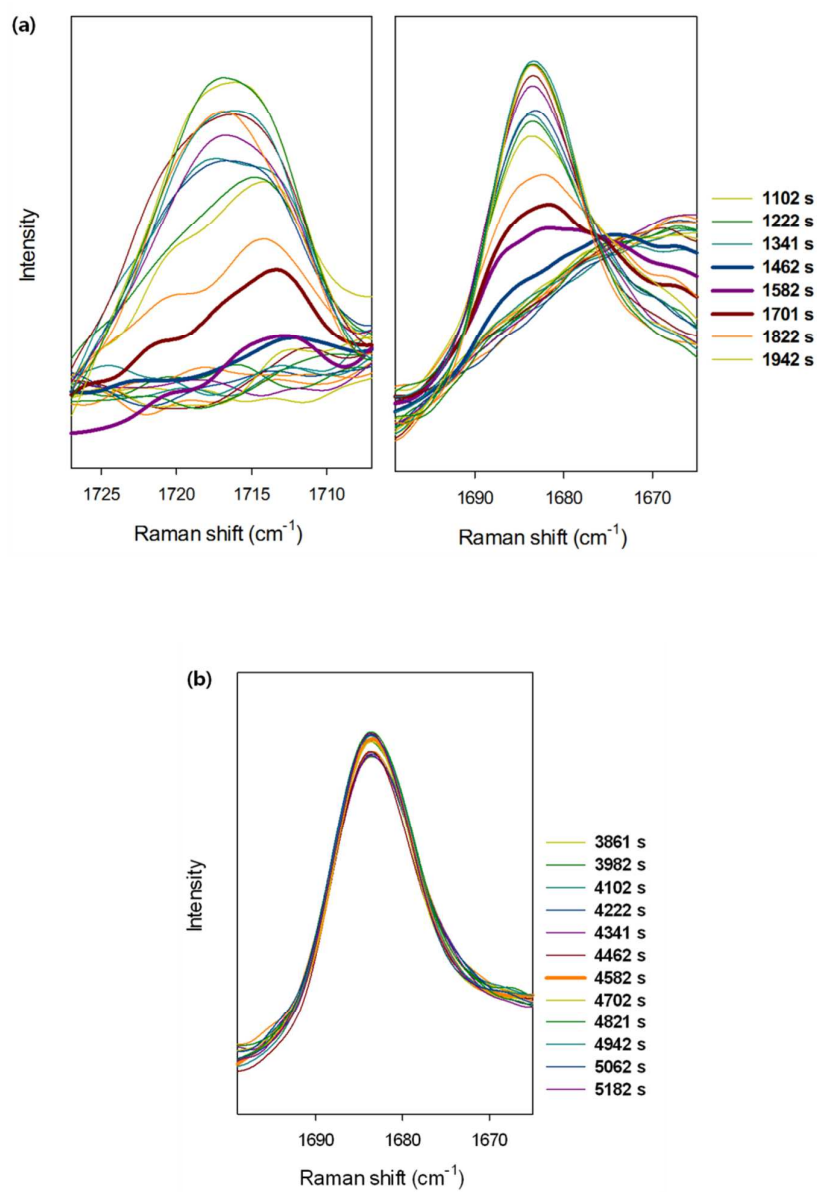
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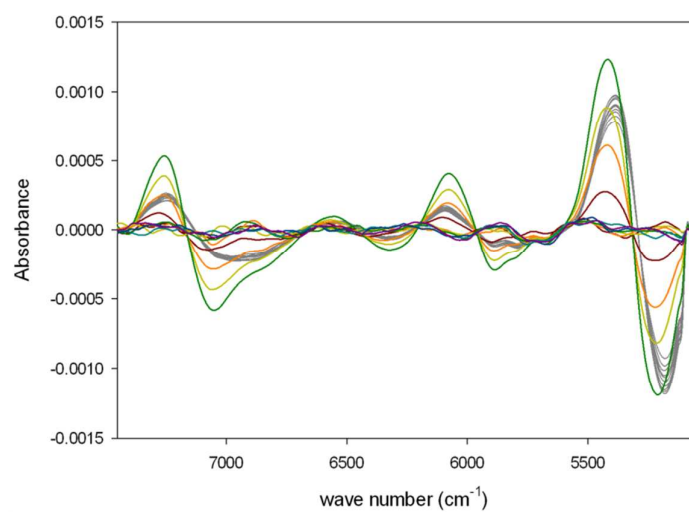
**Figure S-1:** Second derivatives of NIR spectra for IMC  $\alpha$ -form, IMC-SAC co-crystal and mixture phase collected during calibration batches.



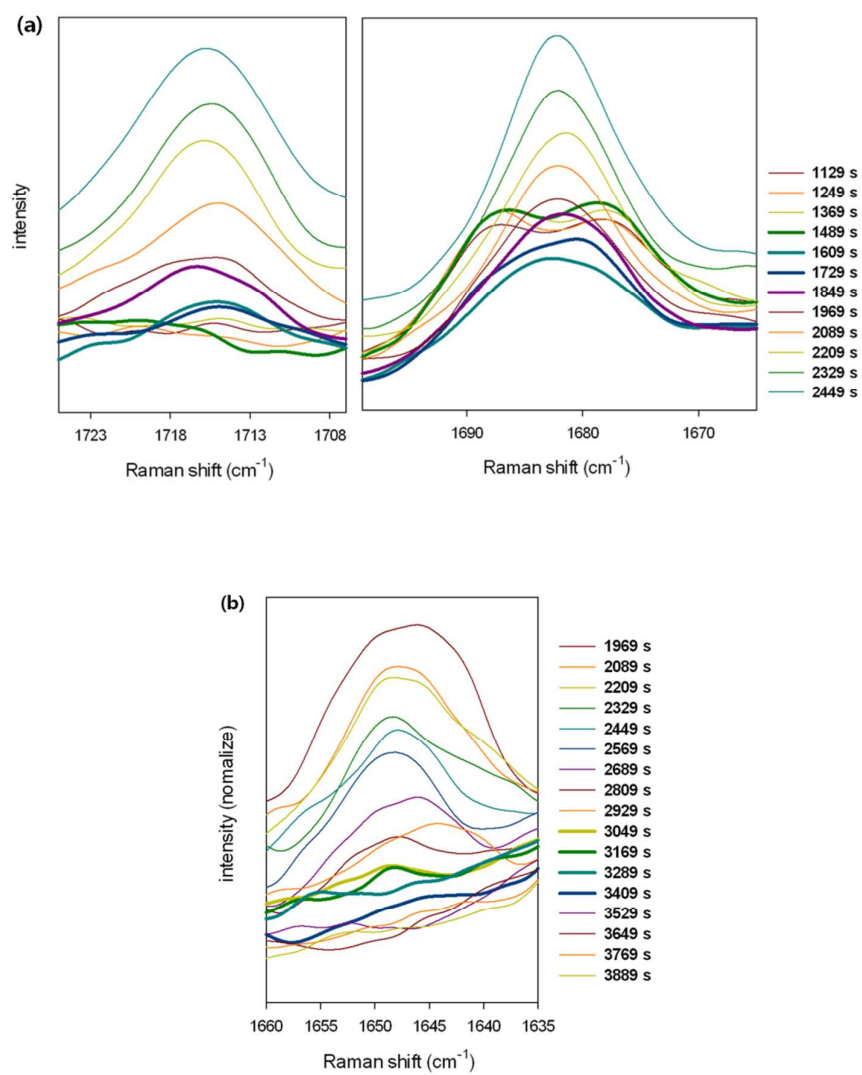
**Figure S-2:** Changes in the Raman peaks around 1717 cm<sup>-1</sup> and 1683 cm<sup>-1</sup> at (a) the nucleation period and (b) the stage of phase equilibrium during Exp 6.



**Figure S-3:** Changes in the Raman peaks around 1717 cm<sup>-1</sup> and 1683 cm<sup>-1</sup> at (a) the nucleation period and (b) the stage of phase equilibrium during Exp 7.



**Figure S-4:** Second derivatives of NIR spectra for IMC-SAC co-crystal (gray lines) and IMC a-form (color lines) collected in the initial stages of nucleation for Exp 6 and Exp 8, respectively.



**Figure S-5:** Changes in Raman peaks (a) around of 1717 cm<sup>-1</sup> and 1683 cm<sup>-1</sup> at the time of co-crystal nucleation and (b) around of 1650 cm<sup>-1</sup> at the stage of the disappearance of IMC  $\alpha$ -form during Exp 8.