SUPPORTING INFORMATION

Challenges in transitioning cocrystals from bench to bedside: Dissociation in prototype drug product environment

Sampada Koranne[§], Anasuya Sahoo[§], Joseph F. Krzyzaniak[‡], Suman Luthra[‡], Kapildev K. Arora*[‡], Raj Suryanarayanan[§]*

[§]Department of Pharmaceutics, College of Pharmacy, University of Minnesota, 9-177 WDH, 308 Harvard Street S.E., Minneapolis, Minnesota 55455, United States of America

[‡]Pfizer Worldwide Research & Development, Groton Laboratories, Groton, CT 06340, United States of America

Corresponding author information
*Raj Suryanarayanan (Sury), PhD
Professor and William and Mildred Peters Endowed Chair
Address: Department of Pharmaceutics, College of Pharmacy
University of Minnesota, 9-177 WDH, 308 Harvard Street S.E.
Minneapolis, MN 55455, USA
Office Phone: 612-624-9626
Fax: 612-626-2125
E-mail: surya001@umn.edu

*Kapildev Arora, PhD
Address: 558 Eastern Point Road, Building 156A Office # 362B
Drug Product Design/Materials Science
Pfizer Worldwide R&D
Groton, CT 06340, USA
Office Phone: 860-441-0412
E-mail: kapildev.arora@pfizer.com

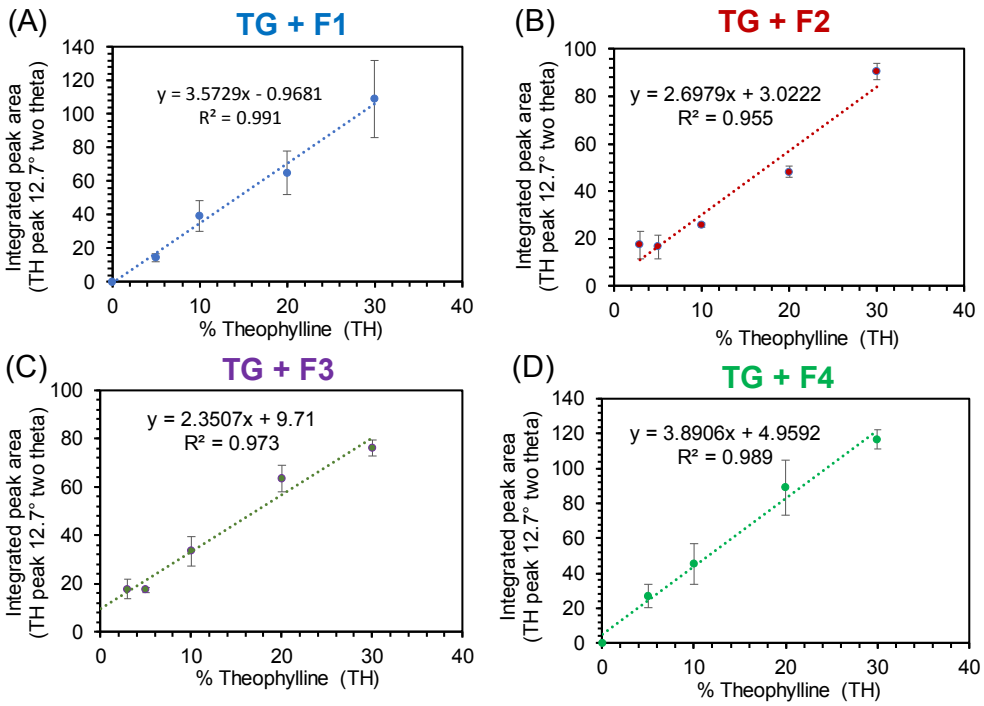

Figure S1. Plot of the intensity of the 12.7° 2θ peak of TH as a function of TH concentration in calibration tablets of (A) TG + F1, (B) TG + F2, (C) TG + F3, and (D) TG + F4.

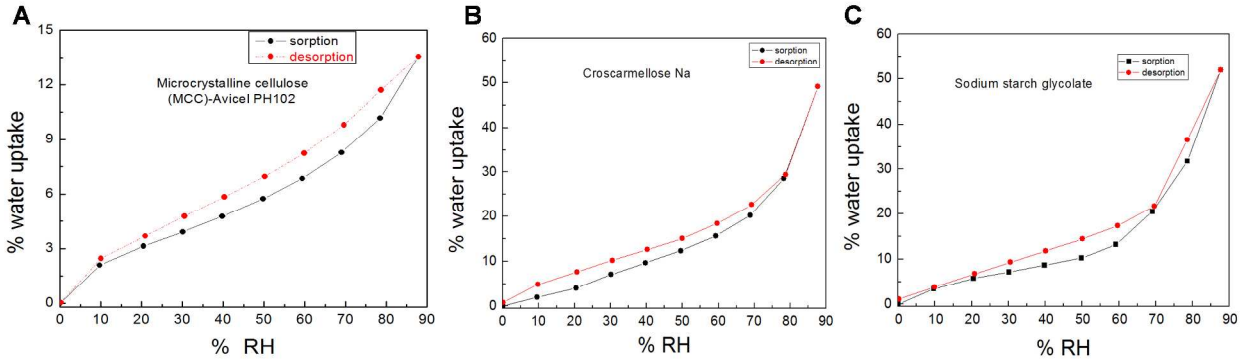

Figure S2. Water sorption-desorption isotherms of (A) microcrystalline cellulose, (B) croscarmellose sodium and, (C) sodium starch glycolate at 25 °C.

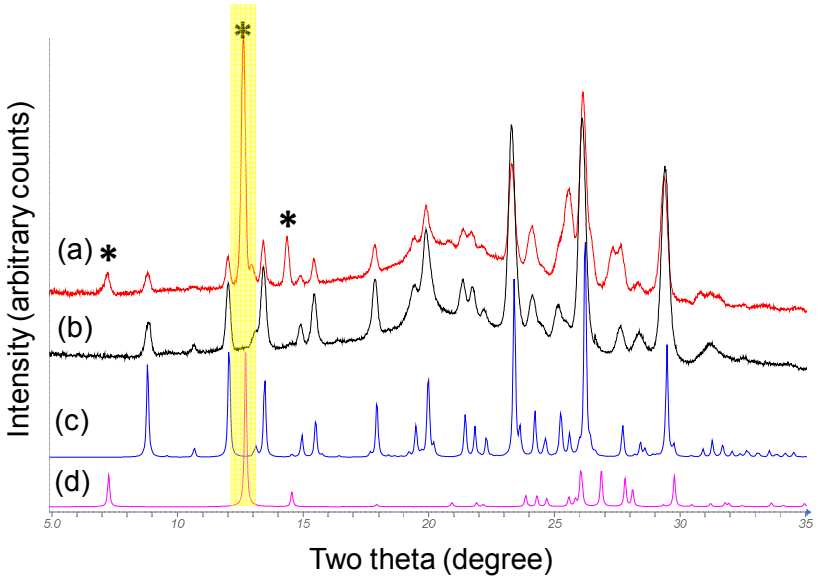

Figure S3. Overlay of XRD patterns of binary compacts of TG prepared with CCS. The XRD patterns of freshly prepared compacts and after storage at 40 °C/75% RH for 1 day are presented in (b) and (a) respectively. The reference patterns of TG cocrystal and theophylline are presented in (c) and (d), respectively.

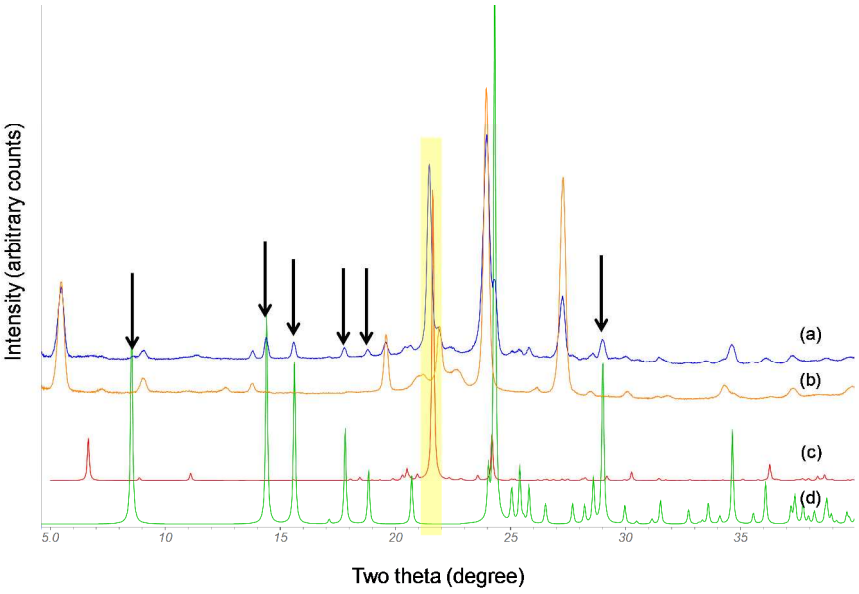

Figure S4. Overlay of XRD patterns of binary compacts of GA (21.15 mg) prepared with MgSt (50.00 mg). The XRD patterns of freshly prepared compacts and after storage at 40 °C/75% RH for two days are presented in (b) and (a) respectively. The reference patterns of stearic acid (CSD ref code STARAC01) and glutaric acid-magnesium-$(H_2O)_4$ complex (CSD ref code NOKFOI), are presented in (c) and (d), respectively. The arrows point several peaks matching with glutaric acid-magnesium $(H_2O)_4$ complex. One characteristic peak for stearic acid observed as a consequence of the reaction is highlighted.