Exploring cocrystal-cocrystal reactivity via liquid-assisted grinding: assembling of racemic and dismantling of enantiomeric cocrystals

Tomislav Friščić, László Fábián, Jonathan C. Burley, William Jones* and W. D. Samuel Motherwell

Supplementary Material

Figure S1. X-ray powder diffraction patterns of cocrystal obtained via liquid-assisted grinding: a) \((\text{theophylline})_2(\text{L-tartaric acid})\) and b) \((\text{theophylline})_2(\text{D-tartaric acid})\).

Figure S2. X-ray powder diffraction patterns of: a) \((\text{theophylline})_2(\text{DL-tartaric acid})\) obtained via liquid-assisted grinding and b) solid obtained by liquid-assisted cocrystal-cocrystal grinding of \((\text{theophylline})_2(\text{L-tartaric acid})\) and \((\text{theophylline})_2(\text{D-tartaric acid})\).

Figure S3. X-ray powder diffraction pattern of \((\text{theophylline})_2(\text{L-tartaric acid})\): a) obtained via liquid assisted grinding and b) calculated from the crystal structure.

Figure S4. X-ray powder diffraction pattern of \((\text{theophylline})_2(\text{DL-tartaric acid})\): a) obtained via liquid assisted grinding and b) calculated from the crystal structure.

Figure S5. X-ray powder diffraction patterns of cocrystal obtained via liquid-assisted grinding: a) \((\text{caffeine})(\text{L-tartaric acid})\) and b) \((\text{caffeine})(\text{D-tartaric acid})\).

Figure S6. X-ray powder diffraction pattern of \((\text{caffeine})(\text{D-tartaric acid})\): a) obtained via liquid assisted grinding and b) calculated from the crystal structure.

Figure S7. X-ray powder diffraction patterns of: a) mixture of caffeine and DL-tartaric acid after liquid-assisted grinding; b) mixture of (caffeine)(L-tartaric acid) and (caffeine)(D-tartaric acid) after liquid-assisted cocrystal-cocrystal grinding and c) physical mixture of caffeine and tartaric acid.
Figure S1. X-ray powder diffraction patterns of cocrystal obtained via liquid-assisted grinding: a) (theophylline)$_2$ (L-tartaric acid) and b) (theophylline)$_2$ (D-tartaric acid).
Figure S2. X-ray powder diffraction patterns of: a) (theophylline)$_2$ (DL-tartaric acid) obtained via liquid-assisted grinding and b) solid obtained by liquid-assisted cocrystal-cocrystal grinding of (theophylline)$_2$ (L-tartaric acid) and (theophylline)$_2$ (D-tartaric acid).
Figure S3. X-ray powder diffraction pattern of (theophylline)$_2$ (L-tartaric acid): a) obtained via liquid assisted grinding and b) calculated from the crystal structure.
Figure S4. X-ray powder diffraction pattern of (theophylline)$_2$ (DL-tartaric acid): a) obtained via liquid assisted grinding and b) calculated from the crystal structure.
Figure S5. X-ray powder diffraction patterns of cocrystal obtained via liquid-assisted grinding: a) (caffeine)(L-tartaric acid) and b) (caffeine)(D-tartaric acid).
Figure S6. X-ray powder diffraction pattern of (caffeine)(D-tartaric acid): a) obtained via liquid assisted grinding and b) calculated from the crystal structure.
Figure S7. X-ray powder diffraction patterns of: a) mixture of caffeine and DL-tartaric acid after liquid-assisted grinding; b) mixture of (caffeine)(L-tartaric acid) and (caffeine)(D-tartaric acid) after liquid-assisted cocrystal-cocrystal grinding and c) physical mixture of caffeine and tartaric acid.