Supplementary Material (ESI) for Chemical Communications

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

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Supplementary Material

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).

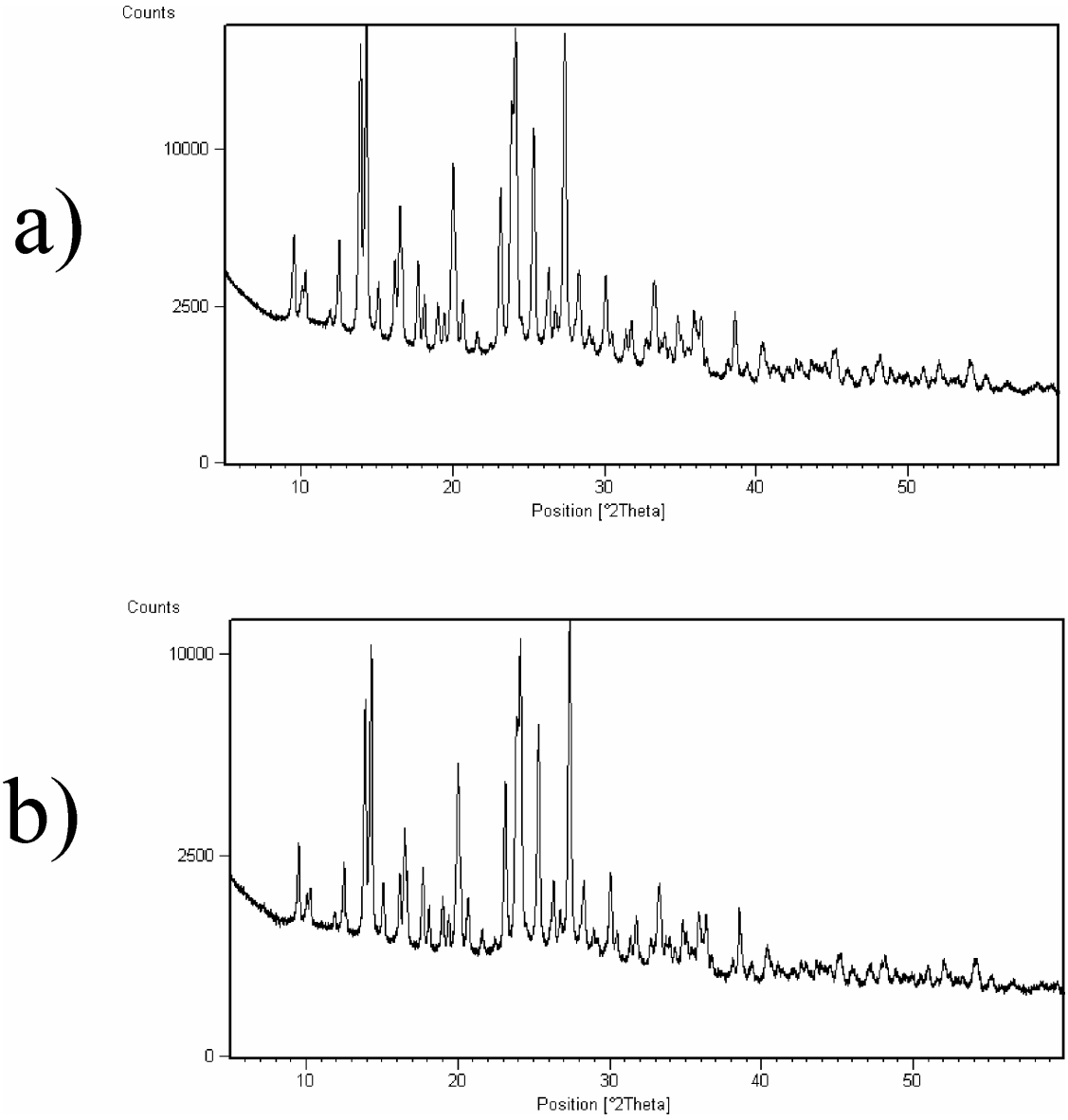
Figure S3. X-ray powder diffraction pattern of (theophylline)$_2$·(L-tartaric acid): a) obtained via liquid assisted grinding and b) calculated from the crystal structure.

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 od (caffeine)·(L-tartaric acid) and (caffeine)·(D-tartaric acid) after liquid-assisted cocrystal-cocrystal grinding and c) physical mixture of caffeine and tartaric acid.



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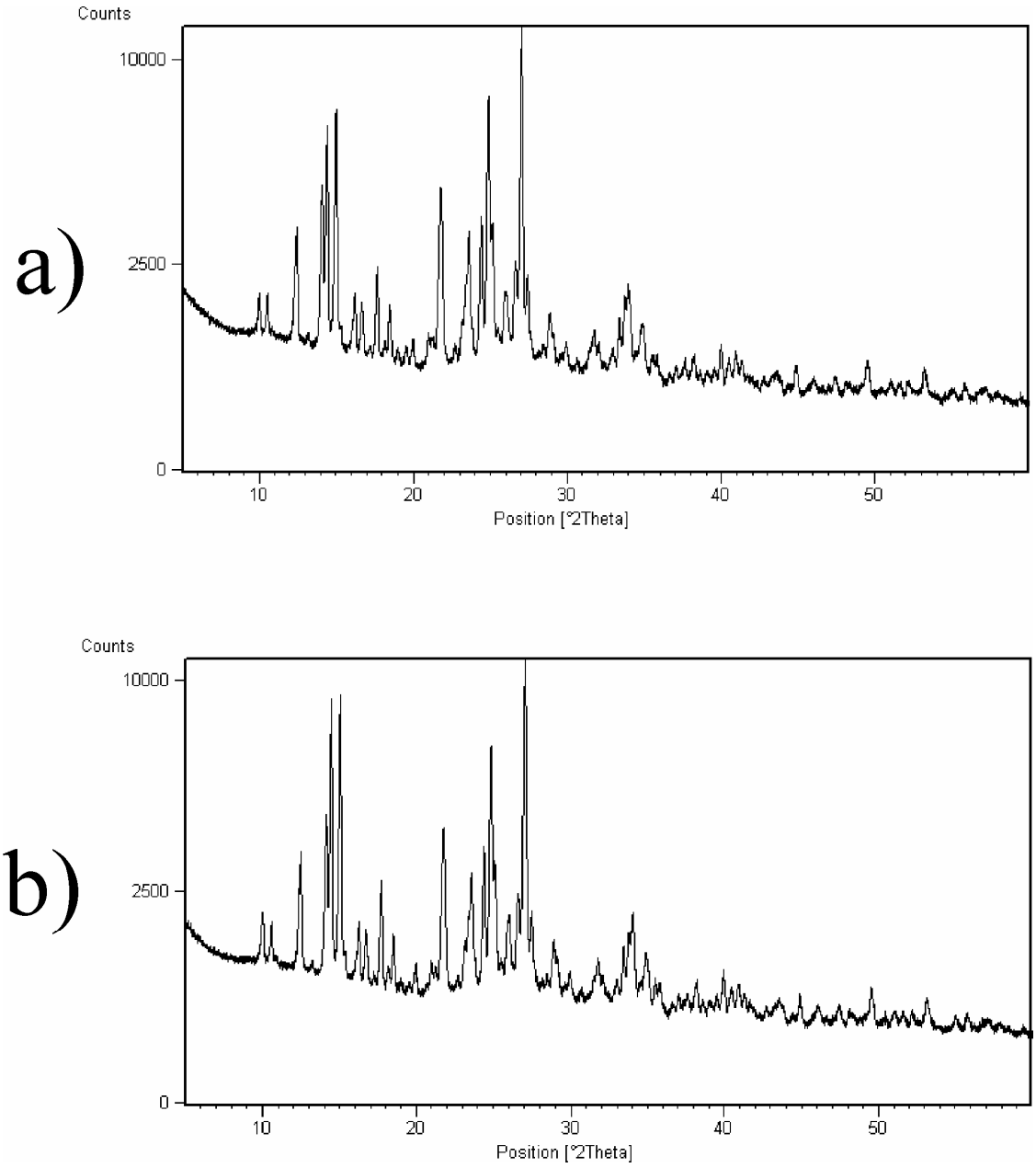
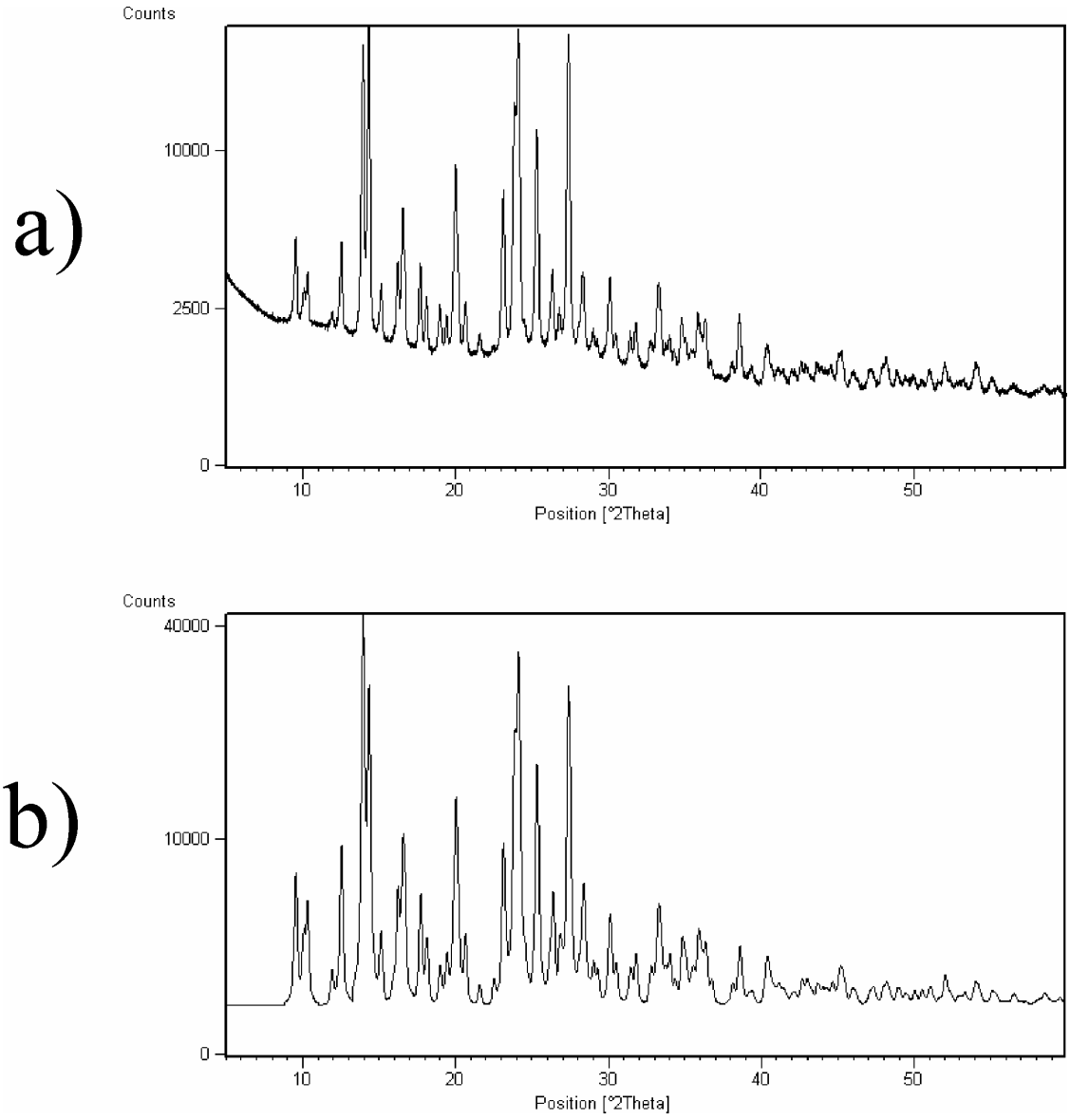


Figure S2. X-ray powder diffraction patterns of: a) (theophylline)$_2$·(DL-tartaric acid) obtained via liquid-assisted grinding and b) solid obtained by liquid-assisted cocrystal-cocrystal grinding of (theophylline)$_2$·(L-tartaric acid) and (theophylline)$_2$·(D-tartaric acid).



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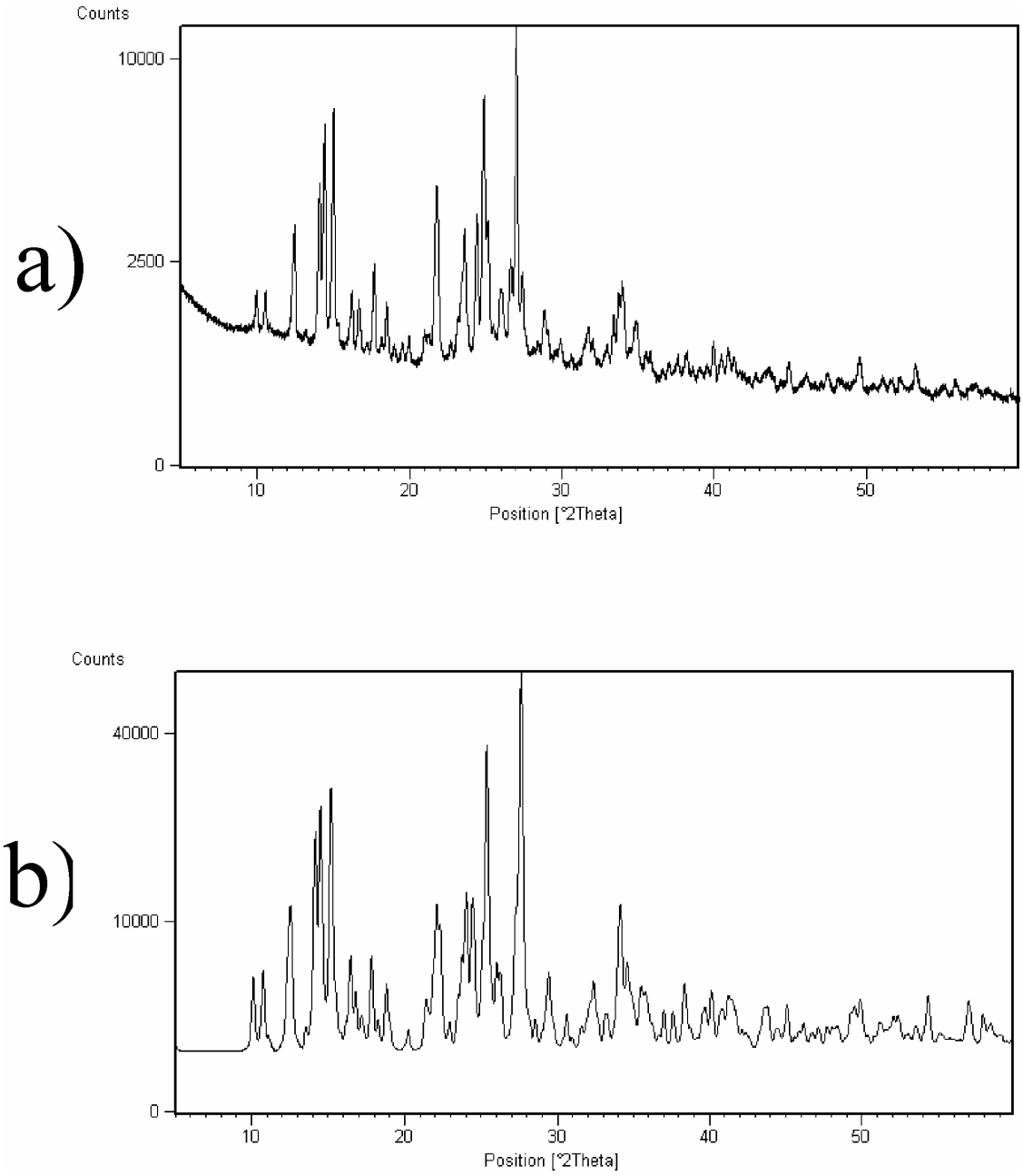


Figure S4. X-ray powder diffraction pattern of (theophylline)$_2$·(DL-tartaric acid): a) obtained via liquid assisted grinding and b) calculated from the crystal structure.

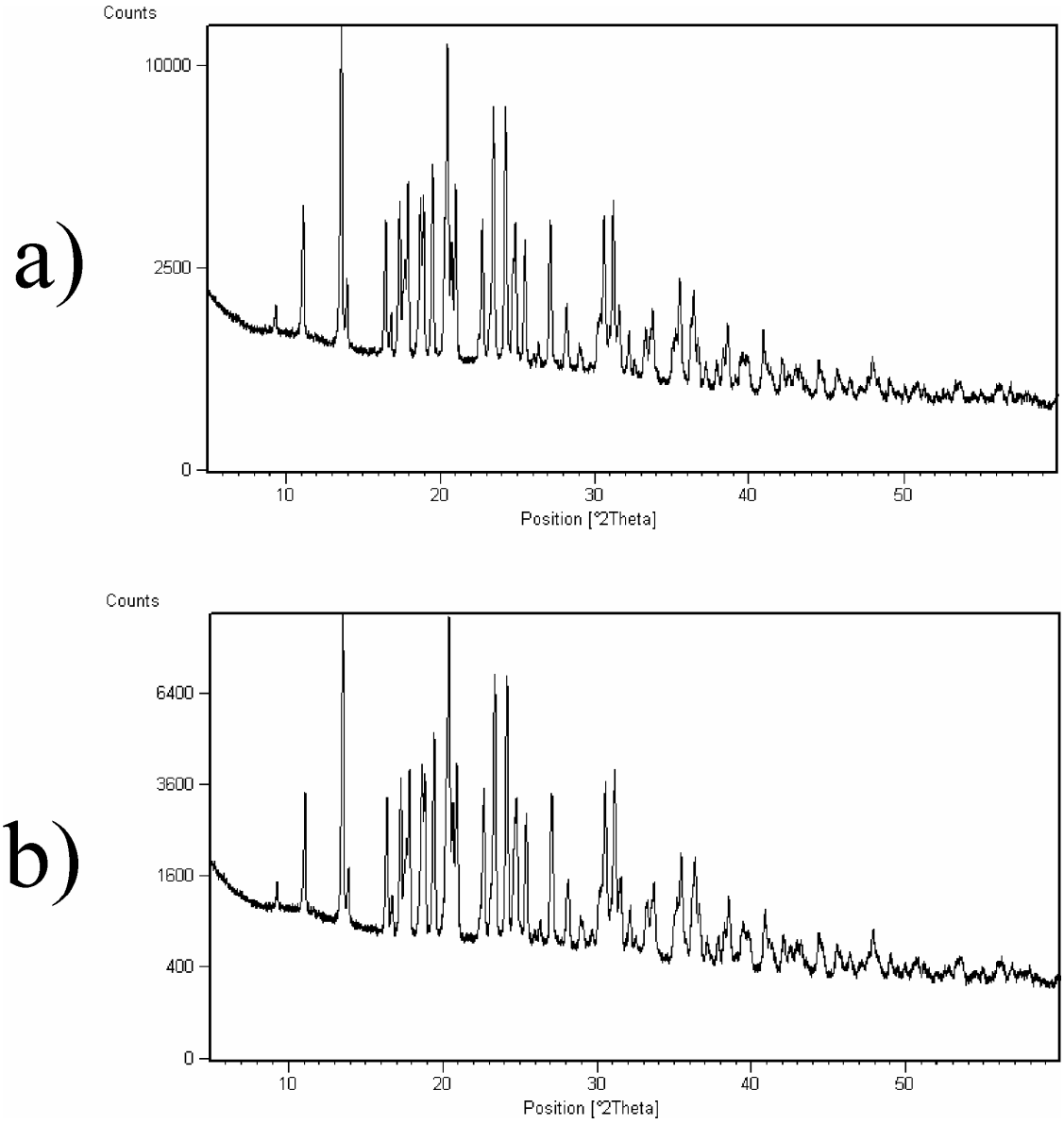
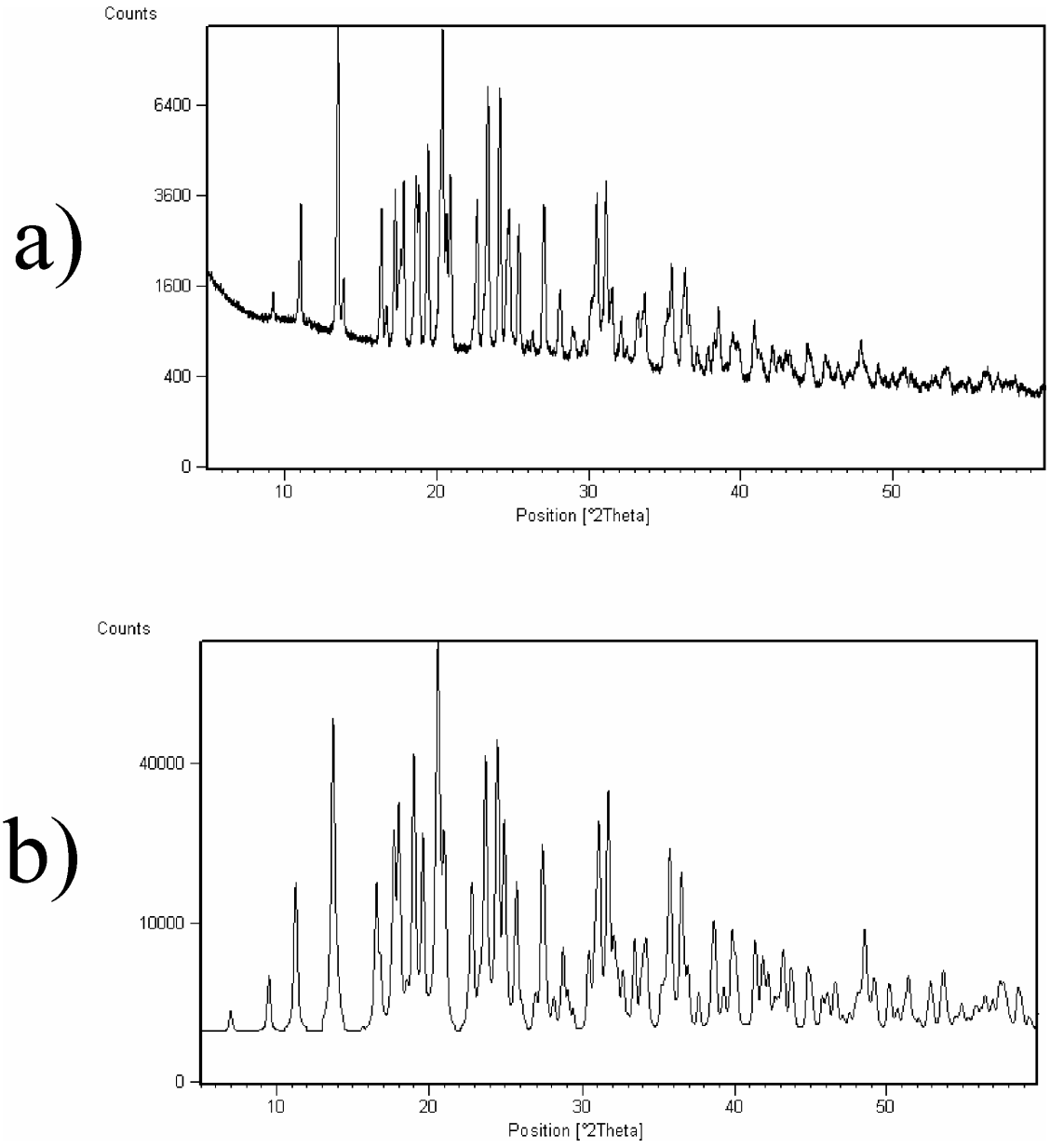


Figure S5. X-ray powder diffraction patterns of cocrystal obtained via liquid-assisted grinding: a) (caffeine)·(L-tartaric acid) and b) (caffeine)·(D-tartaric acid).



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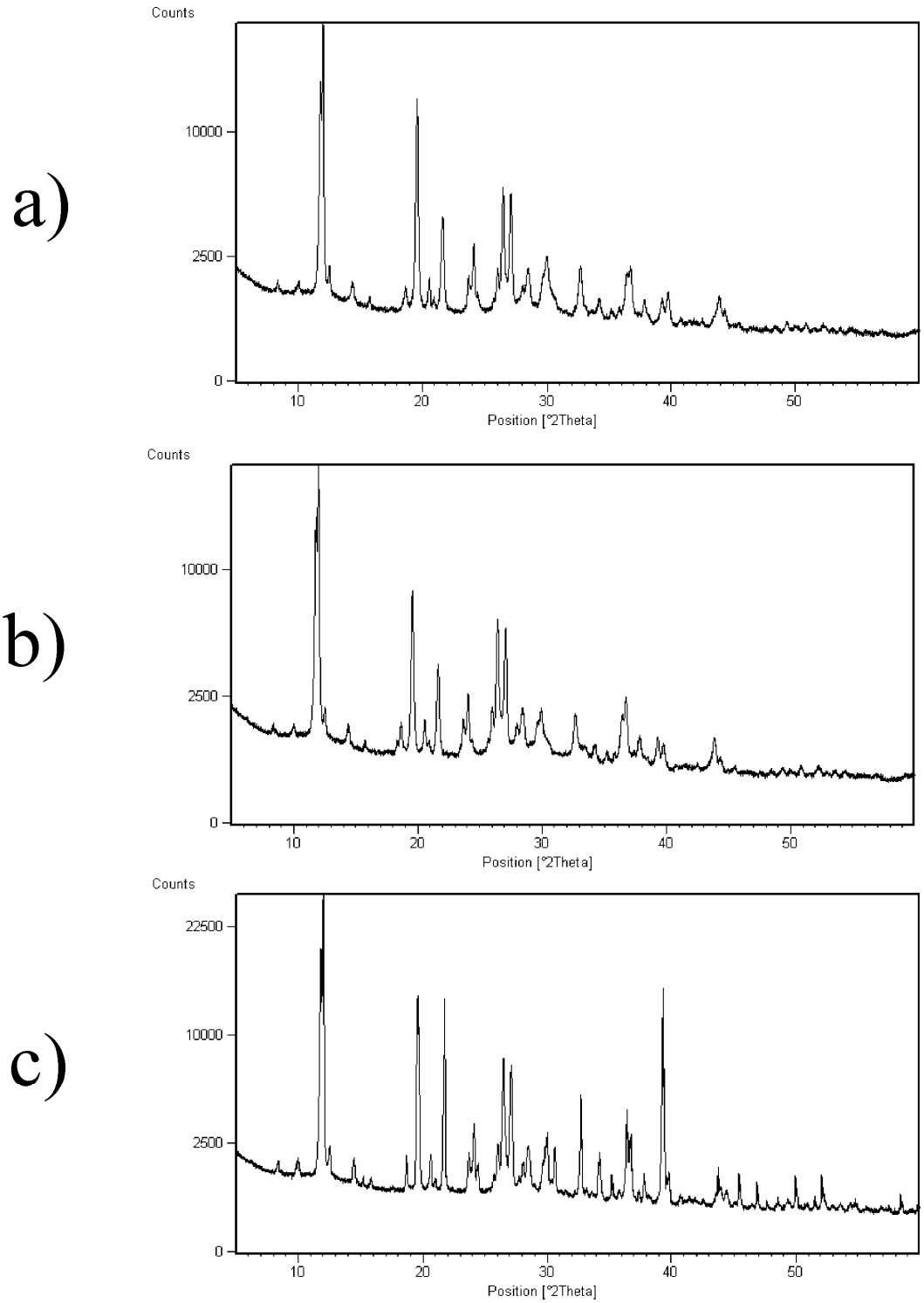

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