Correction to “Rapid polymorph screening on milligram quantities of pharmaceutical material using phonon-mode Raman spectroscopy”, by Sarah Al-Dulaimi, Adeyinka Aina and Jonathan Burley

Correction: outline In a recent publication we outlined the use of low-wavenumber Raman spectroscopy for rapid screening of polymorphism in pharmaceutical materials. We presented data collected on three model systems to illustrate the efficacy of our approach. One of the systems employed was paracetamol, which was selected as it is a well-characterised model system. Because of the well-characterised nature of this model, we did not undertake a thorough and rigorous analysis of our data, but instead based our interpretation on previous work undertaken by one of the authors (JB), published earlier, and supported by a body of other work.

Further, more detailed experiments have indicated that this interpretation, which at the time appeared reasonable, was not valid. As a result the assignments presented in our recent work in CrystEngComm for the Raman spectra of the different solid forms of paracetamol are incorrect. This affects Figure 1 (a and b) and also affects our discussion of the in-situ crystallisation based on data presented in Figure 2a. The main thrust of our paper is unaffected, and results and discussion of the two other systems presented in the work remain valid.

Correction: details In Figure 1 a and 1b, the spectra labelled I and II in fact both correspond to form I, and that labelled III in fact corresponds to form II. A corrected version of Figure 1 is given below, changes have been made to panes a and b only.

Fig. 1 Raman spectra of the solid forms of: paracetamol (a,b); FFA (c,d); imipramine hydrochloride (e,f). A =
amorphous.

Likewise, in Figure 2a of our original publication, the spectra were incorrectly ascribed to a series of transformations from amorphous to form III to form II. With the benefit of a thorough review of the data and more detailed experiments, it has become clear that these data in fact correspond to a transformation sequence amorphous to form II (not III), then to form I (not II).

**Conclusion:** Our error in assuming reproducibility of the crystallisation pathway of amorphous paracetamol was compounded by the fact that we collected spectra at 10 °C intervals, which meant that unambiguous identification of polymorphic forms via their melting points was not possible. The collection of data every 10 °C was due to technical constraints in place at the time of the original experiments which have since been resolved. To avoid any similar mistake in future, we have updated our screening protocol to ensure that spectra are collected every 1 °C in future, and are employing statistical tests rather than visual observation to differentiate between spectra. We also hope that the recent development of density-functional theory to a level whereby confident peak assignments can be made for solid-state Raman spectra 5 will prove invaluable in future work. We apologise wholeheartedly for any confusion caused to the readership of CrystEngComm.

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**References:**