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Capecitabine from X-ray powder synchrotron data. Corrigendum

Jan Rohlicek,[a]* Michal Husak,[a] Ales Gavenda,[b] Alexandr Jegorov,[c] Bohumil Kratochvil[a] and Andy Fitch[d]

[a]Department of Solid State Chemistry, ICT Prague, Technicka 5, Prague, Czech Republic, [b]IVAX Pharmaceuticals s.r.o., R&D, Opava, Czech Republic, [c]Pharmaceuticals Research and Development, Branisovska 31, Ceske Budejovice, Czech Republic, and [d]ID31 Beamline, ESRF, 6 rue Jules Horowitz, BP 220, F-38043 Grenoble Cedex, France. *Correspondence e-mail: rohlicej@vscht.cz

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In the paper by Rohlicek *et al.* [*Acta Cryst.* (2009), E**65**, o1325–o1326], one H atom was placed incorrectly.

Following our powder-diffraction study of capecitabine (Rohlicek *et al.*, 2009), Malińska *et al.* (2014) published the crystal structure of the same molecule based on single-crystal data. Although they modelled the wrong enantiomer [as was pointed out by Kratochvil *et al.* (2016)], the structures are very similar after inverting the single-crystal structure, including

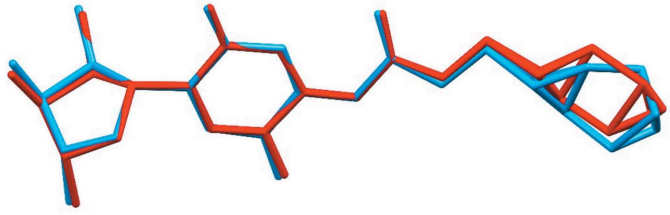
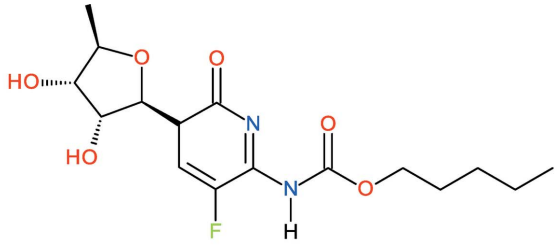
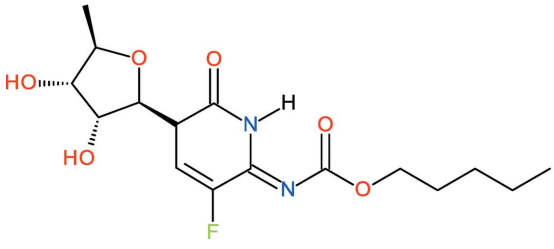


Figure 1
Overlay of the capecitabine molecular structures arising from powder diffraction (blue) and from single-crystal diffraction data (red). Only non-H atoms are shown for clarity.



(a)



(b)

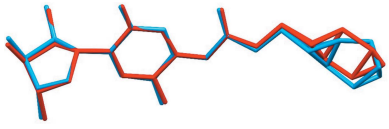


Figure 2
Schemes for the tautomeric forms of capecitabine (*a*) assumed in the powder-diffraction study and (*b*) established in the single-crystal study of Malinska *et al.* (2014).

the disordered part of the molecule (Fig. 1). Since single-crystal diffraction is more sensitive to H atoms than powder diffraction, Malinska *et al.* (2014) were able to locate the H atoms directly. This indicated a different tautomeric form of capecitabine to that assumed in our study, and as they pointed out, we had therefore placed one H atom wrongly.

In our defence, in the powder study, we placed the H atoms geometrically according to a reasonable chemical structure for capecitabine, which shows the tautomeric H atom attached to the N atom of the carbamate group and the plausible formation of an intermolecular N—H···O hydrogen bond. As shown by Malińska *et al.* (2014), the H atom is actually located on the N atom of the pyrimidine ring (Fig. 2), thereby forming an intramolecular N—H···O link.

With respect to the fact that structure solution from powder diffraction data is based on the proposed molecular structure, readers should beware of the incorrectly placed H atom in Rohlicek *et al.* (2009) and they should be also beware of the wrong enantiomer in a single-crystal study of Malińska *et al.* (2014).

References

Kratochvil, B., Husak, M., Korotkova, E. I. & Jegorov, A. (2016). *Chem. Listy*, **110**, 40–47.

Malińska, M., Krzecyński, P., Czerniec-Michalik, E., Trzcińska, K., Cmoch, P., Kutner, A. & Woźniak, K. (2014). *J. Pharm. Sci.* **103**, 587–593.

Rohlicek, J., Husak, M., Gavenda, A., Jegorov, A., Kratochvil, B. & Fitch, A. (2009). *Acta Cryst.* E**65**, o1325–o1326.