CrystEngComm



CORRECTION

View Article Online



Cite this: CrystEngComm, 2024, 26, 5830

Correction: Quadrupolar NMR crystallography guided crystal structure prediction (QNMRX-CSP)

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DOI: 10.1039/d4ce90117g

rsc.li/crystengcomm

Correction for 'Quadrupolar NMR crystallography guided crystal structure prediction (QNMRX-CSP)' by Austin A. Peach et al., CrystEngComm, 2024, 26, 4782-4803, https://doi.org/10.1039/D3CE01306E.

The authors regret that there was an error in Fig. 5 of the manuscript which showed results for N,N-dimethylglycine HCl rather than for metformin HCl. The correct Fig. 5 is as shown here:

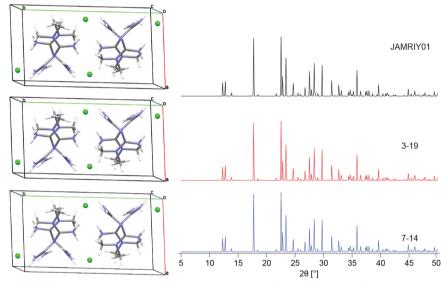


Fig. 5 A comparison of the DFT-D2* geometry-optimized structural model of metformin HCl derived from its known crystal structure (JAMRIY01) with two (from the set of four) validated structural models from S4 blind tests, 3-19 and 7-14, with $\Gamma_{\rm FFG}$ = 0.059 and 0.067 MHz, $E_{\rm lat}$ = 0.067 and 0 kJ mol^{-1} , R = 0.962 and 0.086%, and RMSD = 0.007 and 0.007 Å, respectively.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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