



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

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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>.

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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:

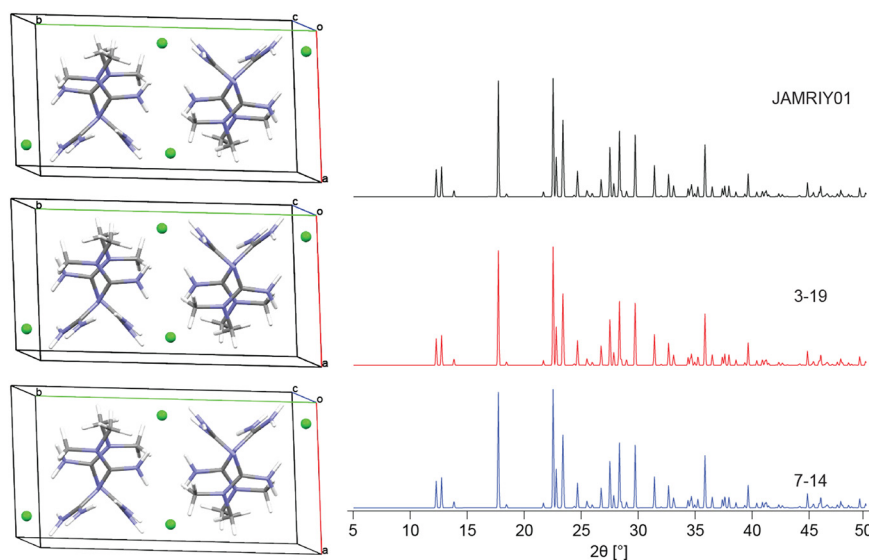


Fig. 5 A comparison of the DFT-D2* geometry-optimized structural model of metformin HCl derived from its known crystal structure (JAMRIY01) with two (from the set of four) validated structural models from S4 blind tests, 3–19 and 7–14, with $I_{\text{EFG}}^{\text{C}} = 0.059$ and 0.067 MHz, $E_{\text{lat}} = 0.067$ 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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