



Cite this: *CrystEngComm*, 2024, 26, 5830

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

Austin A. Peach,^{ab} Carl H. Fleischer III,^{ab} Kirill Levin,^c Sean T. Holmes,^{ab}
Jazmine E. Sanchez^{ab} and Robert W. Schurko^{*ab}

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:

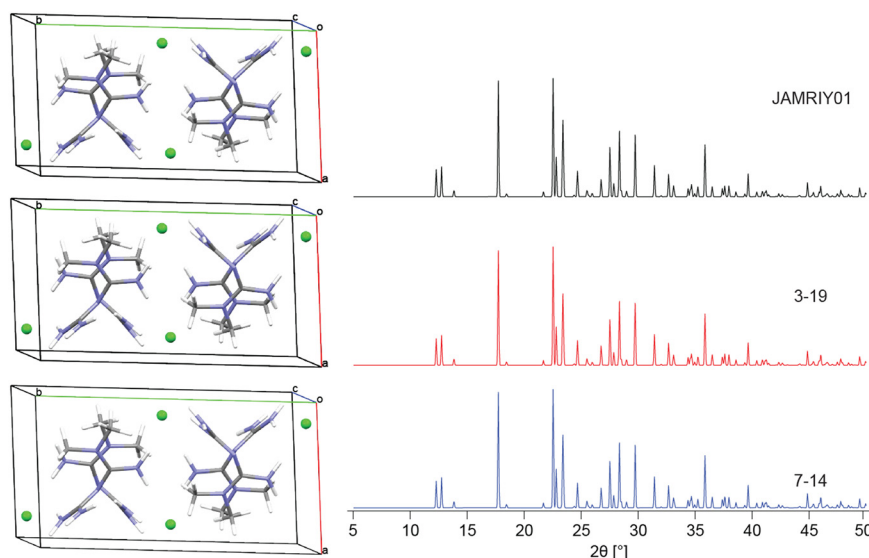


Fig. 5 A comparison of the DFT-D2* geometry-optimized structural model of metformin HCl derived from its known crystal structure (JAMRIY01) with two (from the set of four) validated structural models from S4 blind tests, 3–19 and 7–14, with $\Gamma_{\text{EFG}} = 0.059$ and 0.067 MHz, $E_{\text{lat}}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

^a Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, USA. E-mail: rschurko@fsu.edu; Tel: +1 850 645 8614

^b National High Magnetic Field Laboratory, Tallahassee, FL 32310, USA

^c Department of Chemistry and Biochemistry, McGill University, Montreal, Quebec, Canada

