Digital Discovery



CORRECTION

View Article Online
View Journal | View Issue



Cite this: Digital Discovery, 2025, 4,

Correction: Distortion/interaction analysis *via* machine learning

Samuel G. Espley, page 3 Samuel S. Allsop, page 3 David Buttar, page 5 Simone Tomasi page 3 and Matthew N. Grayson page 4 Simone Tomasi page 5 Simone Tomasi

DOI: 10.1039/d5dd90005k rsc.li/digitaldiscovery

Correction for 'Distortion/interaction analysis *via* machine learning' by Samuel G. Espley *et al., Digital Discovery*, 2024, **3**, 2479–2486, https://doi.org/10.1039/D4DD00224E.

It has come to the authors' attention that there is a small error in the data repository for this paper. In the process of putting the data archive together, there was a copy error of one file rendering the dataset incomplete. We have now added the missing structure, in a new instance of the data archive at DOI: https://doi.org/10.15125/BATH-01480.

We have also updated the data collection method description on the data archive to better reflect the procedure used.

We have ensured that this error happened after the research for the paper was completed and therefore, the data, results, and conclusions presented in the paper are unaffected.

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

^{*}Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, UK. E-mail: M.N.Grayson@bath.ac.uk

^bData Science and Modelling, Pharmaceutical Sciences, R&D, AstraZeneca, Macclesfield, UK

^cChemical Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, UK