nature COMMUNICATIONS

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https://doi.org/10.1038/s41467-020-17423-x OPEN

Author Correction: Representation of molecular structures with persistent homology for machine learning applications in chemistry

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Correction to: *Nature Communications* https://doi.org/10.1038/s41467-020-17035-5, published online 26 June 2020.

In the original version of this article, some text was missing from the legends of Figure 5 and Figure 6.

The legend of Figure 5 originally read:

"CO_2 interaction energy distribution shown as horizontal violin plots for the first, second, and third active-learning steps. The height of the shape shows the frequency of occurrences.."

The correct version states:

"CO_2 interaction energy distribution shown as horizontal violin plots for the first, second, and third active-learning steps. **a** CM, **b** BoB, **c** SOAP, and **d** PI. The height of the shape shows the frequency of occurrences…"

This has been corrected in both the PDF and HTML version of the article.

The legend of Figure 6 originally read**:**

"Predicted CO_2 and N_2 interaction energies (in kcal mol^{-1}) for all molecules in the GDB-9 database using four molecular representation models. Only the model that utilized the PI molecular representation …"

The correct version states:

"Predicted CO_2 and N_2 interaction energies (in kcal mol^{-1}) for all molecules in the GDB-9 database using four molecular representation models. **a** CM, **b** BoB, **c** SOAP, and **d** PI. Only the model that utilized the PI molecular representation."

This has been corrected in both the PDF and HTML version of the article.

Published online: 14 July 2020