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Correction: Characterizing the ligand-binding affinity toward SARS-CoV-2 Mpro via physics- and knowledge-based approaches

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Correction for 'Characterizing the ligand-binding affinity toward SARS-CoV-2 Mpro via physics- and knowledge-based approaches' by Son Tung Ngo et al., *Phys. Chem. Chem. Phys.*, 2022, <https://doi.org/10.1039/d2cp04476e>.

The authors would like to make a correction to Fig. 8 in the published version of the article. The corrected figure is shown below.

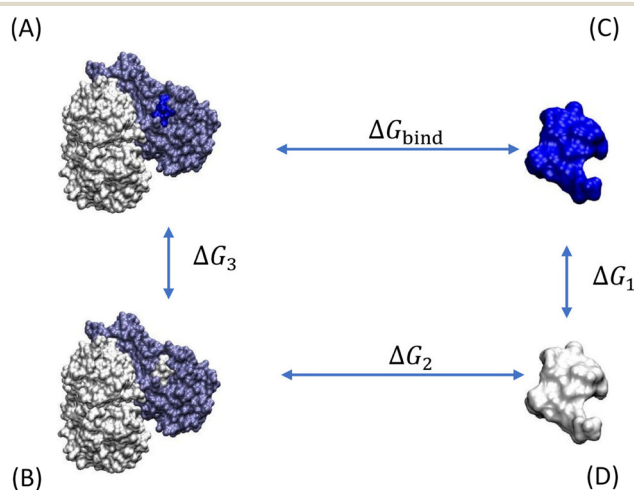


Fig. 8 Schematic illustration of the calculation of the binding free energy between SARS-CoV-2 Mpro and a ligand via the FEP approach.¹¹⁵ (A) The full-interaction state of a ligand with Mpro and solvation. (B) The noninteraction state of a ligand with Mpro and solvation. (C) The full-interaction state of a ligand with solvation. (D) The noninteraction state of a ligand with solvation. The solvent is not shown for clarity.

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

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