PCCP



View Article Online

CORRECTION



Cite this: Phys. Chem. Chem. Phys., 2023, 25, 878

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

Son Tung Ngo,*^{ab} Trung Hai Nguyen,^{ab} Nguyen Thanh Tung,^{cd} Van V. Vue,^e Minh Quan Pham*^{df} and Binh Khanh Mai^g

DOI: 10.1039/d2cp90233h

rsc.li/pccp

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.

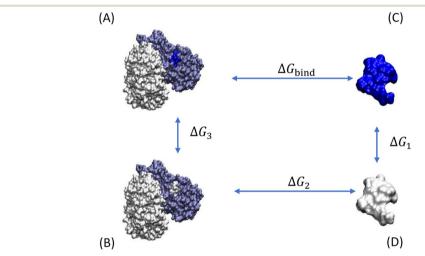


Fig. 8 Schematic illustration of the calculation of the binding free energy between SARS-CoV-2 Mpro and a ligand *via* the FEP approach.¹¹⁵ (A) The full-interaction state of a ligand with Mpro and solvation. (B) The noninteraction state of a ligand with Mpro and solvation. (C) The full-interaction state 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.

^a Laboratory of Theoretical and Computational Biophysics, Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City, Vietnam.

^fInstitute of Natural Products Chemistry, Vietnam Academy of Science and Technology, Hanoi, Vietnam

E-mail: ngosontung@tdtu.edu.vn

^b Faculty of Pharmacy, Ton Duc Thang University, Ho Chi Minh City, Vietnam

^c Institute of Materials Science, Vietnam Academy of Science and Technology, Hanoi, Vietnam. E-mail: minhquanaries@gmail.com

^d Graduate University of Science and Technology, Vietnam Academy of Science and Technology, Hanoi, Vietnam

^e NTT Hi-Tech Institute, Nguyen Tat Thanh University, Ho Chi Minh City, Vietnam

^g Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, USA