Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information: Unveiling the molecular mechanism of SARS-CoV-2 main protease inhibition from 137 crystal structures using algebraic topology and deep learning

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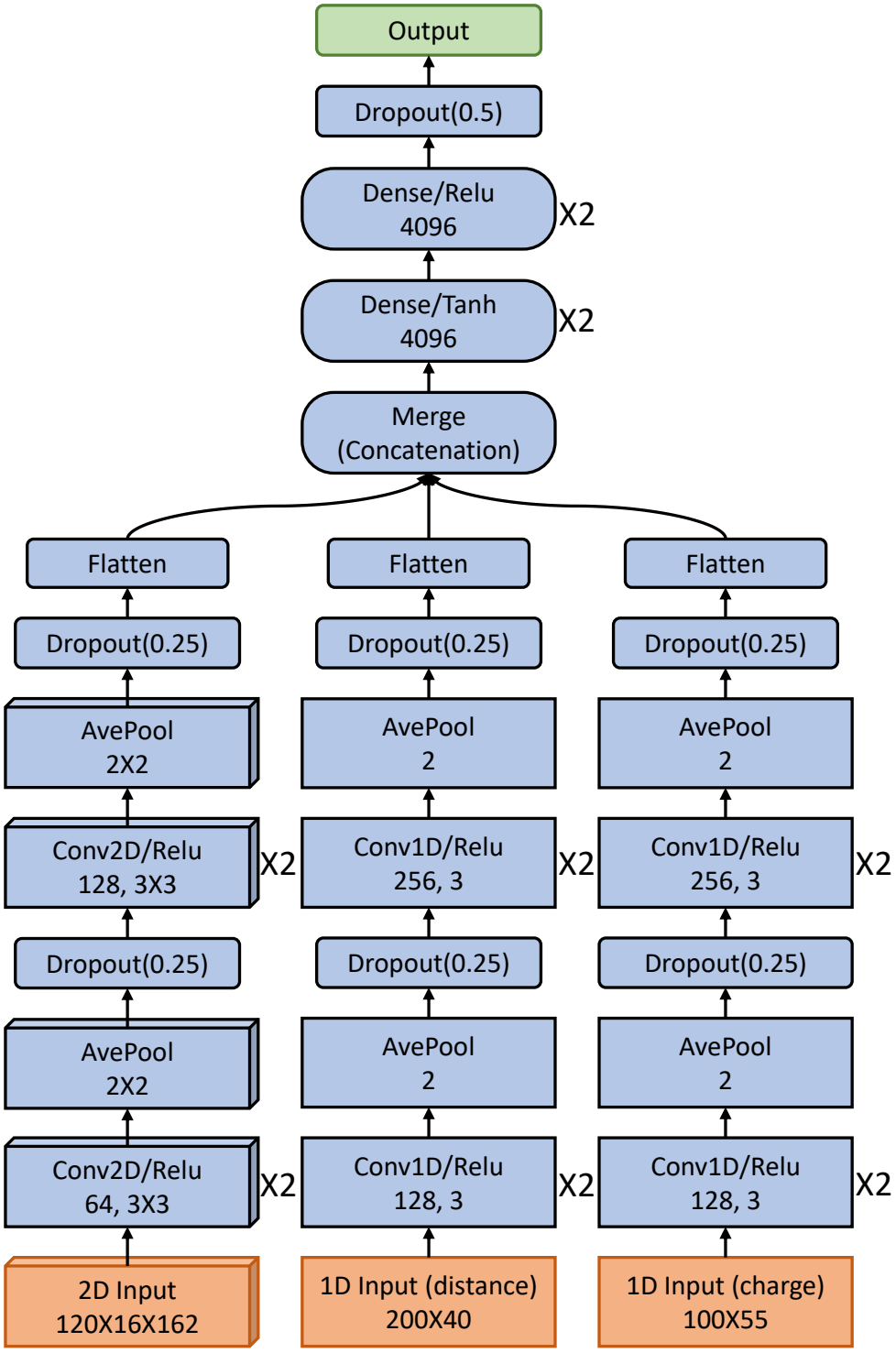

Figure S1: The network architecture for MathDL[1] used for SARS-CoV-2 main protease inhibition binding energy prediction. At each convolution layer, number on the left indicates the number of filters, and number on the right stands for the filter size. Number of layer repetition is specified by "$\times n$" sign on the right side of the layer. In the dense players, number of neurons and type of activation functions are presented.

References

[1] Z. X. Cang, L. Mu, and G. W. Wei, “Representability of algebraic topology for biomolecules in machine learning based scoring and virtual screening ,” *PLOS Computational Biology*, vol. 14(1), pp. e1005929, https://doi.org/10.1371/journal.pcbi.1005929, 2018.