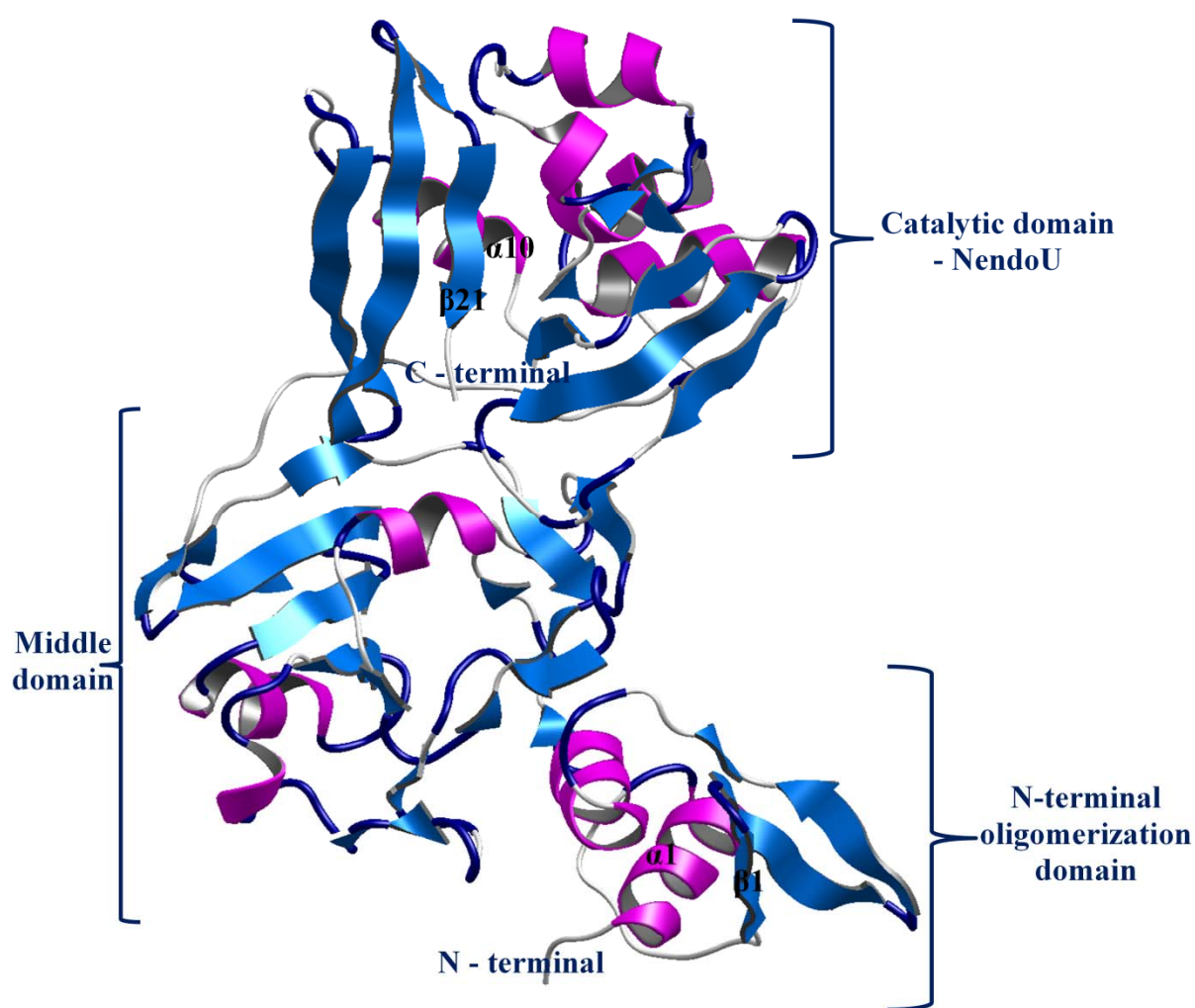


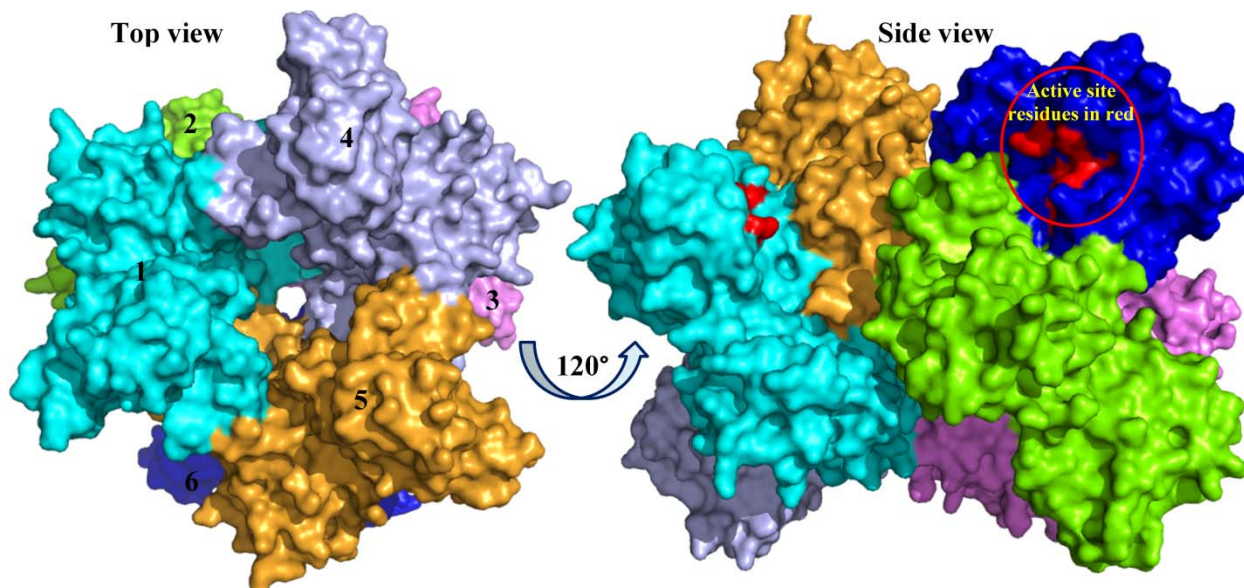
# Pharmacoinformatics approach based identification of potential Nsp15 endoribonuclease modulators for SARS-CoV-2 inhibition

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## *Supplementary data*



**Figure S1.** Cartoon representation of the secondary structural elements of SARS-CoV-2 Nsp15 monomer (PDB ID: 6W01) [1]. Schematic diagram showing the N-terminal domain, middle domain, and C-terminal domain.



**Figure S2.** Surface view representation of Nsp15 hexamer (PDB ID: 2RHB) [2]. Each subunit displayed in distinct colors (1-6). The active site amino acid residues are highlighted in red colored.

## References

- [1] Y. Kim, R. Jedrzejczak, N.I. Maltseva, M. Wilamowski, M. Endres, A. Godzik, K. Michalska, A. Joachimiak, Crystal structure of Nsp15 endoribonuclease NendoU from SARS-CoV-2, *Protein Sci.* 29 (2020) 1596-1605. <https://doi.org/10.1002/pro.3873>.
- [2] K. Bhardwaj, S. Palaninathan, J.M.O. Alcantara, L.L. Yi, L. Guarino, J.C. Sacchettini, C.C. Kao, Structural and functional analyses of the severe acute respiratory syndrome coronavirus endoribonuclease Nsp15, *J. Biol. Chem.* 283 (2008) 3655-3664. <https://doi.org/10.1074/jbc.M708375200>.