# Supporting Information

## In silico identification of novel SARS-COV-2 2′-O-methyltransferase (nsp16) inhibitors: Structure-based virtual screening, molecular dynamics simulation and MM-PBSA approaches

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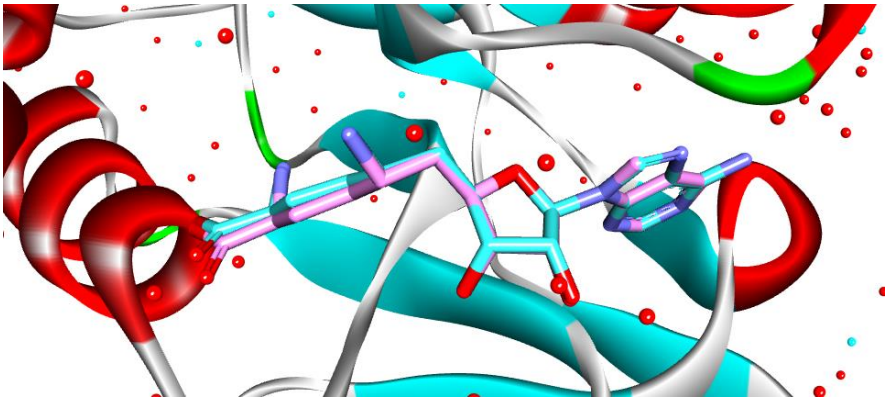
**A.**



**B.**

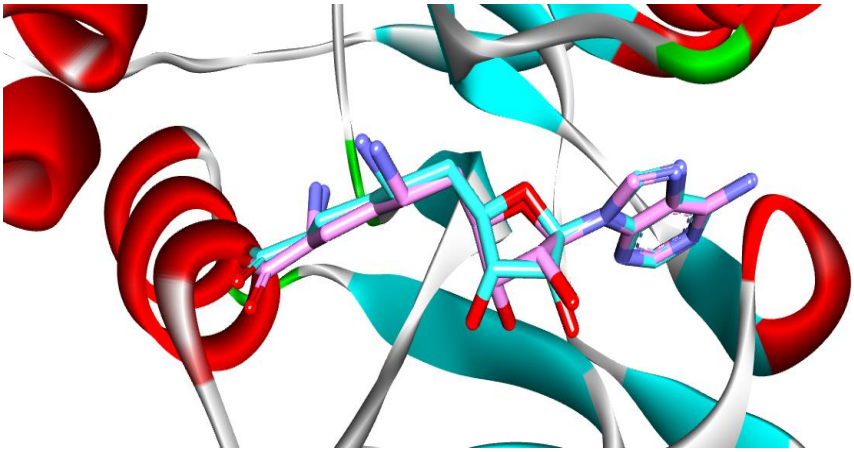


**Figure S1**. Superimposition between co-crystalized (Cyan) and re-docked pose (Pink) of Sinefungine (A) in presence of water (B) in absence of water showing nearly the same binding. mode.

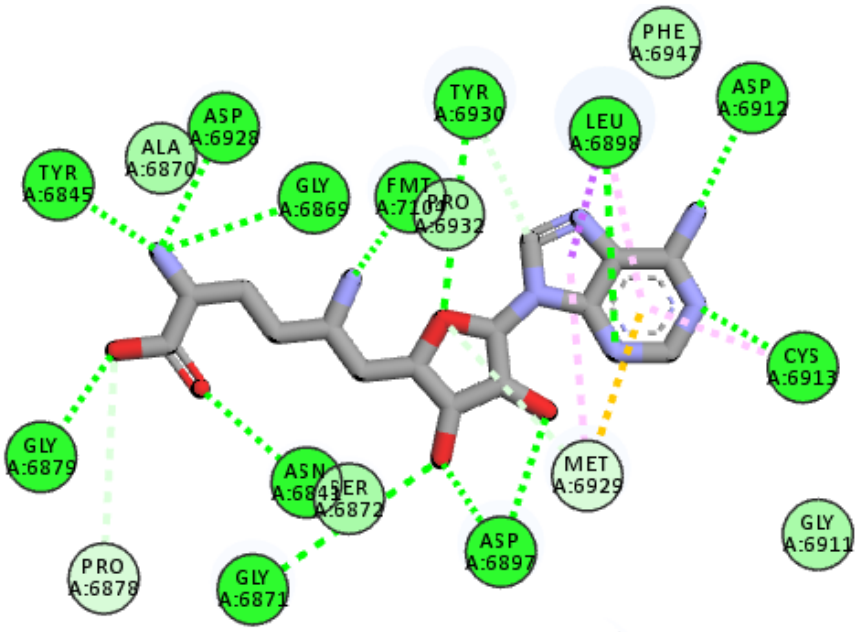



**Figure S2.** Binding of Sinefungine to SARS COV-2 2′-o-methyltransferase (nsp16) before equilibration showing many interactions that may be either significant or not.

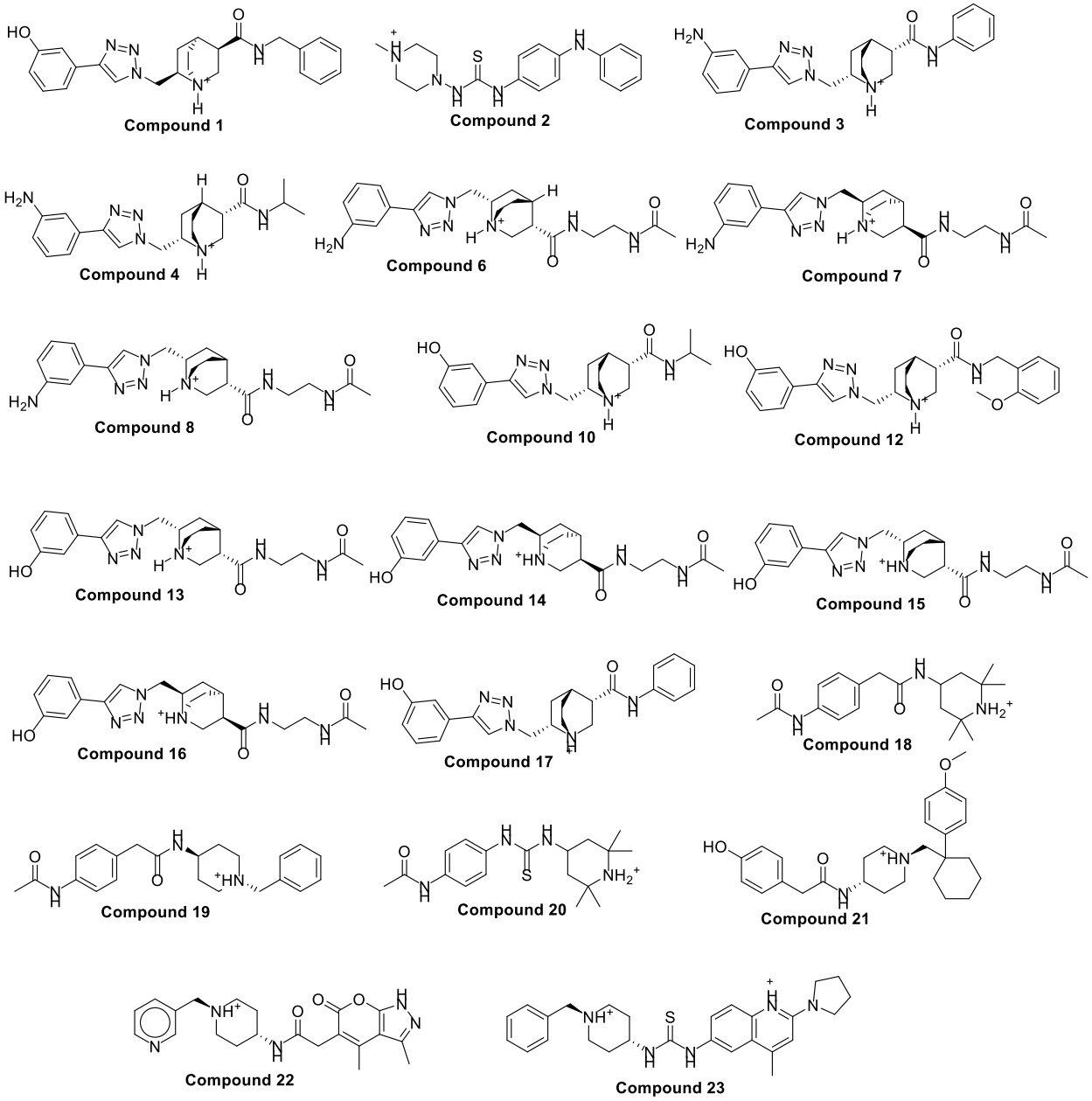



**Figure S3.** Chemical structures for compounds passed the pharmacophore filter and were further screened through docking-based virtual screening.