Supporting information

Targeting C-terminal helical bundle of NCOVID19 Envelope (E) protein

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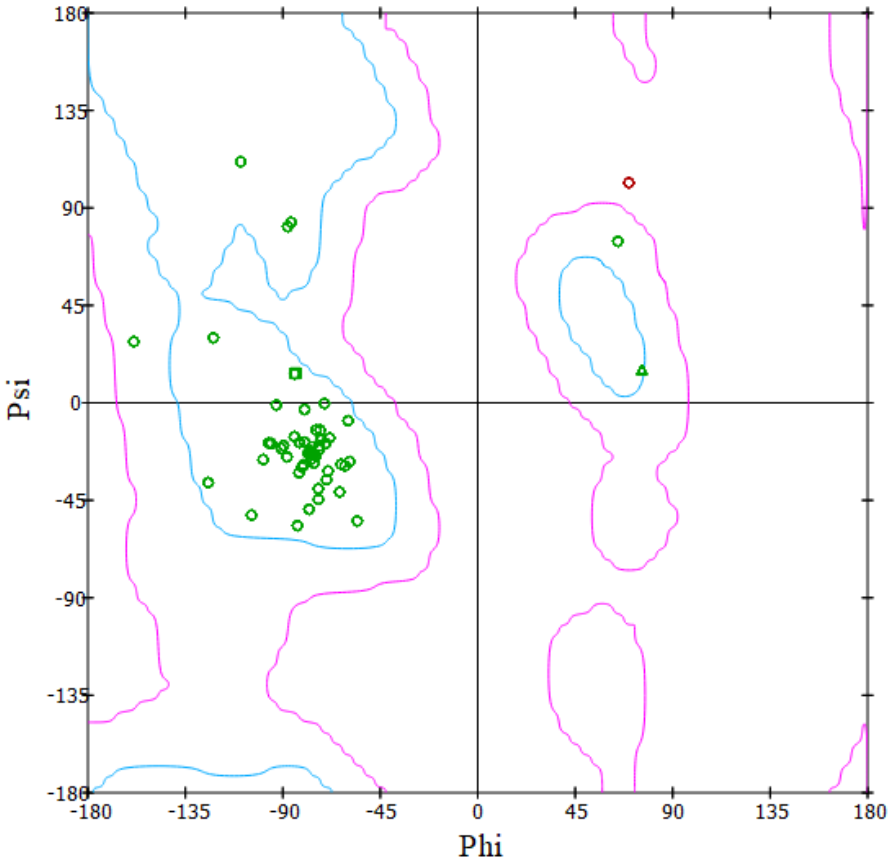
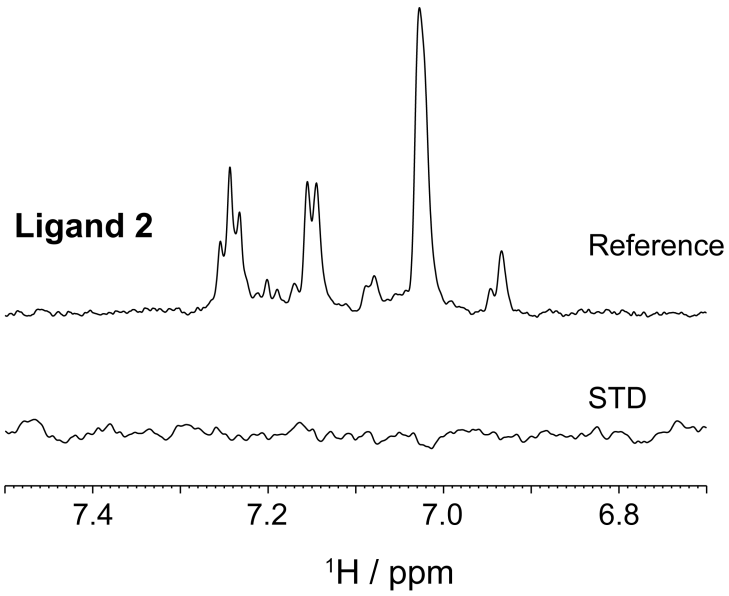
Table 1: Thirteen ligands were mapped to the NCOVID19 envelope protein based pharmacophore from the recently reported 133 FDA drug molecules that were able to inhibit SARS-CoV2 infection in Vero cell line screen. These ligands are used as internal control in our study.

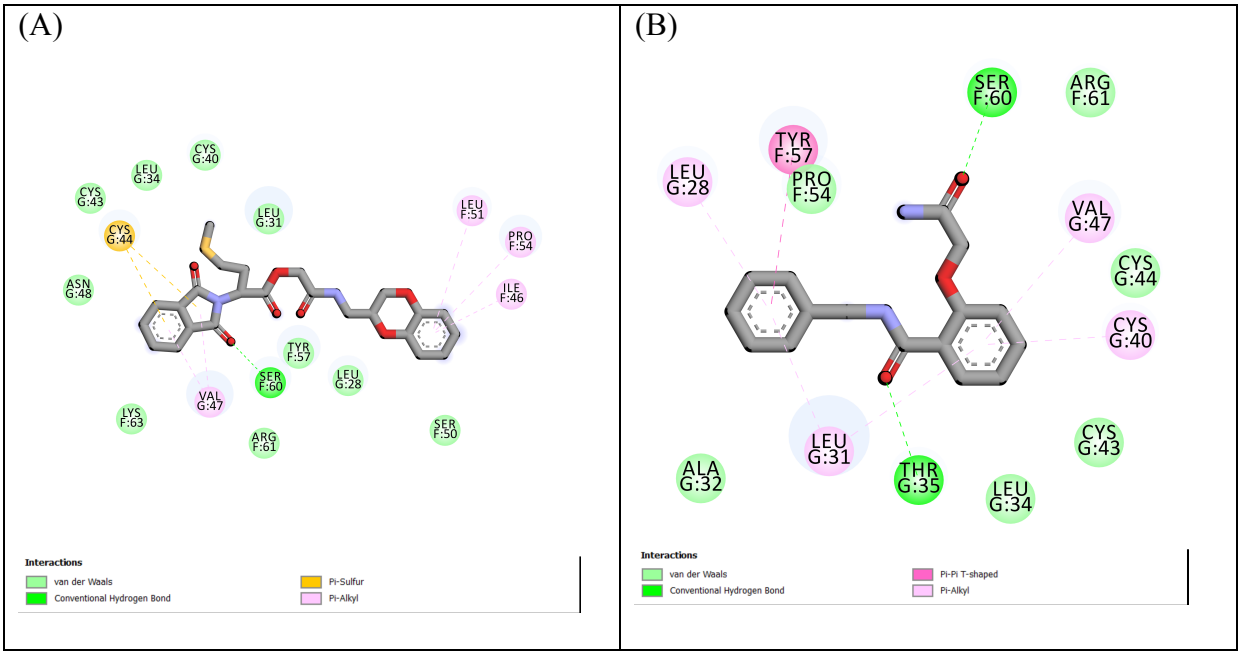
Sl.NO	**chembl_id**	**chembl_pref_name**	**FitValue**
1	CHEMBL36342	OCTENIDINE HYDROCHLORIDE	4.40544
2	CHEMBL4303781	None	3.87139
3	CHEMBL729	LOPINAVIR	3.84105
4	CHEMBL4303661	None	3.82407
5	CHEMBL4065616	REMDESIVIR	3.67963
6	CHEMBL1751	DIGOXIN	3.51426
7	CHEMBL95431	CARBOXYAMIDOTRIAZOLE	3.44995
8	CHEMBL4303781	None	3.42836
9	CHEMBL4303522	None	3.40554
10	CHEMBL1208572	SALINOMYCIN	3.40129
11	CHEMBL46286	OMACETAXINE MEPESUCCINATE	3.39726
12	CHEMBL264241	ANIDULAFUNGIN	3.3379
13	CHEMBL4303448	None	3.12001
14	CHEMBL3786230	None	2.46894



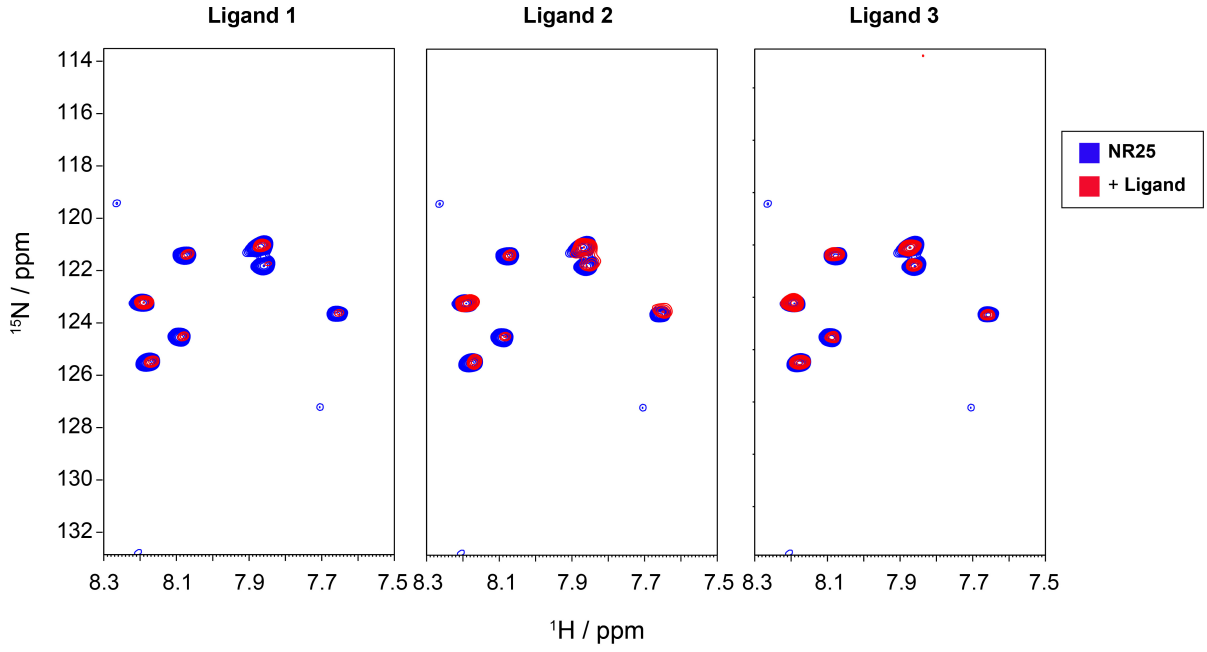
Supplementary Figure 1: Ramachandran Plot showing most of the residues are in most favoured regions and only one residue in generously allowed region (~l), suggesting good stereochemical quality of the homology model.



Supplementary Figure 2: STD NMR spectrum of **Ligand 2** binding to NCOVID 19 E protein. No STD signal of **ligand 2** was observed upon binding to E protein, signifying non-binder.



Supplementary Figure 3: 2D interaction plot for the interaction between the lead compounds and C-terminal domain of E protein (A) ZINC23221929, (B) ZINC06220062.



Supplementary Figure 4: 2D ^{1}H-^{15}N HSQC spectra of NR25 in the absence (blue colour) and presence (red colour) of ligands **1**, **2** or **3**. The experiment was performed using Bruker Avance III 700 MHz using RT probe and at 298 K.