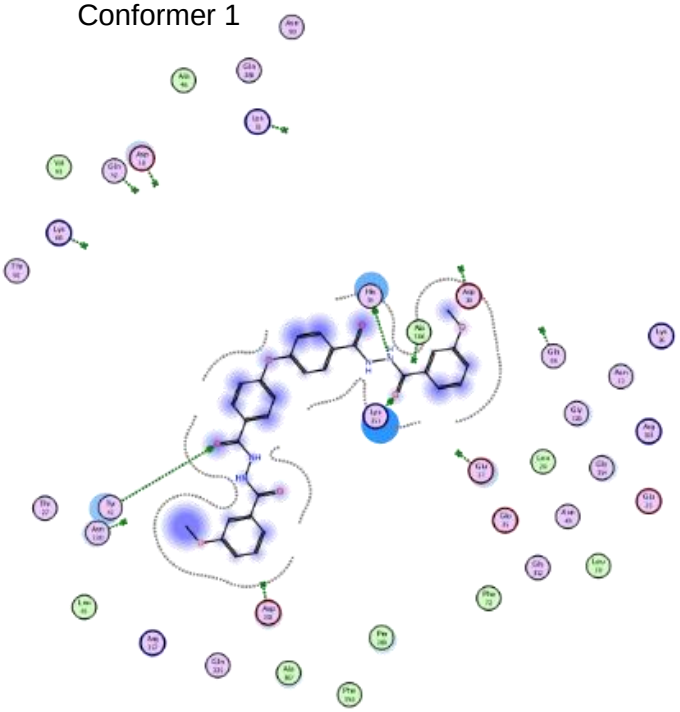
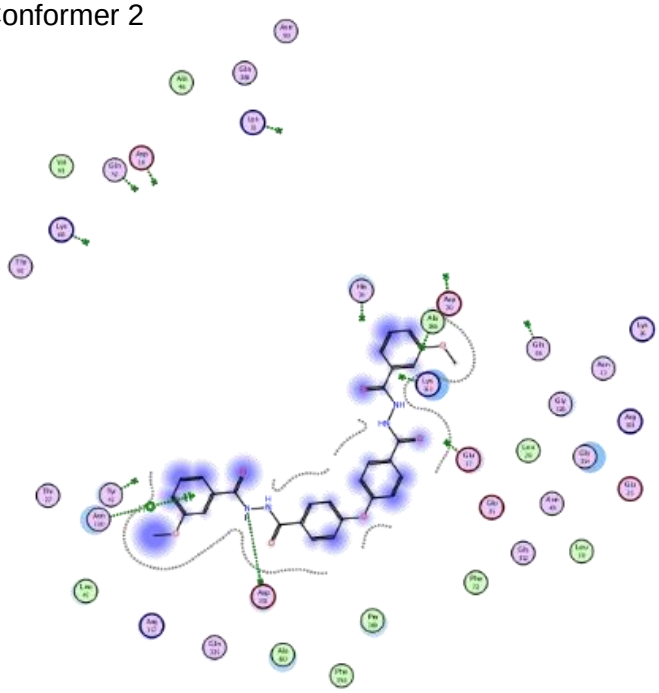
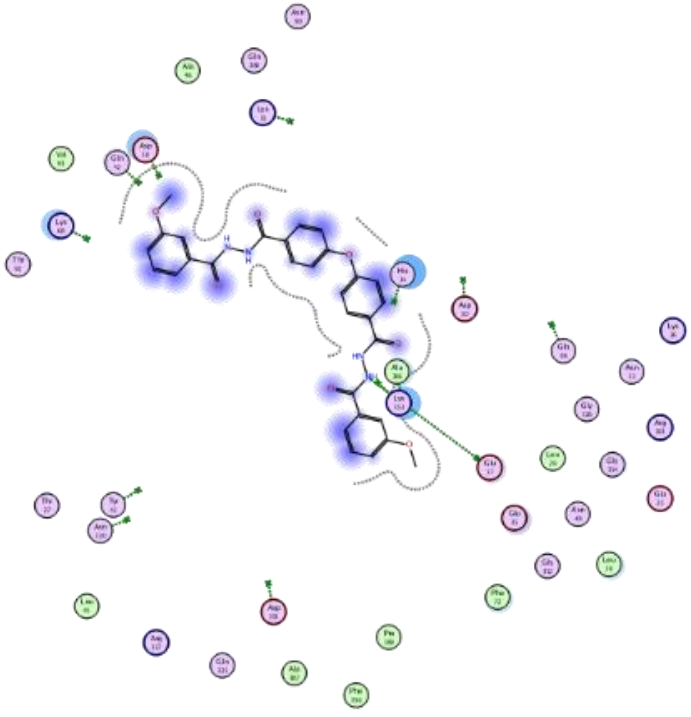
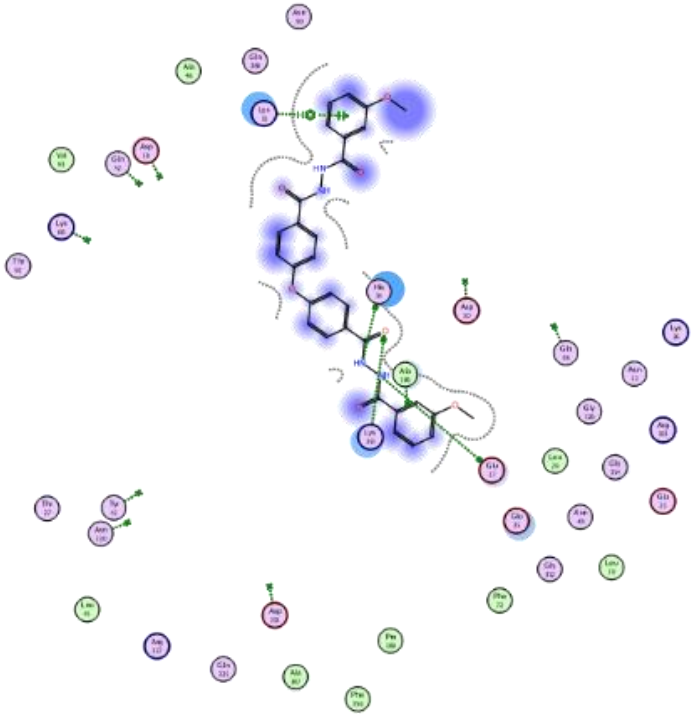
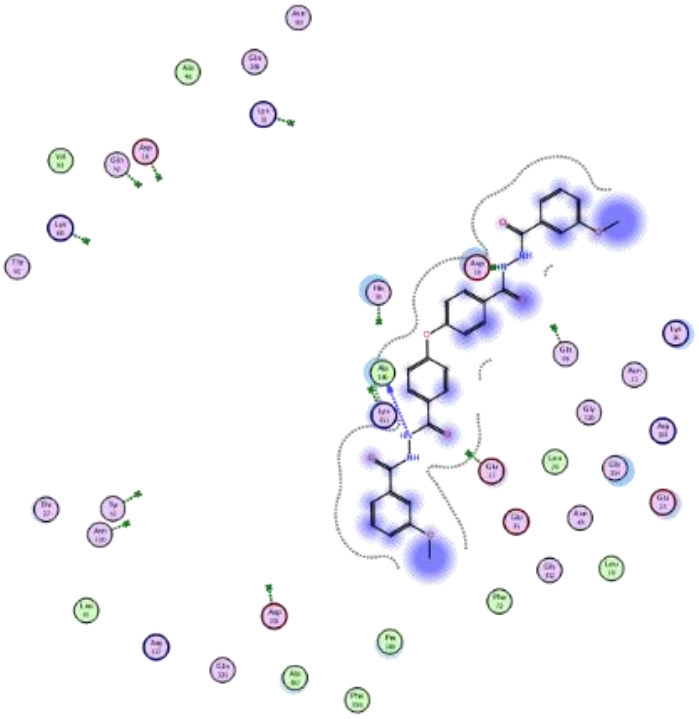
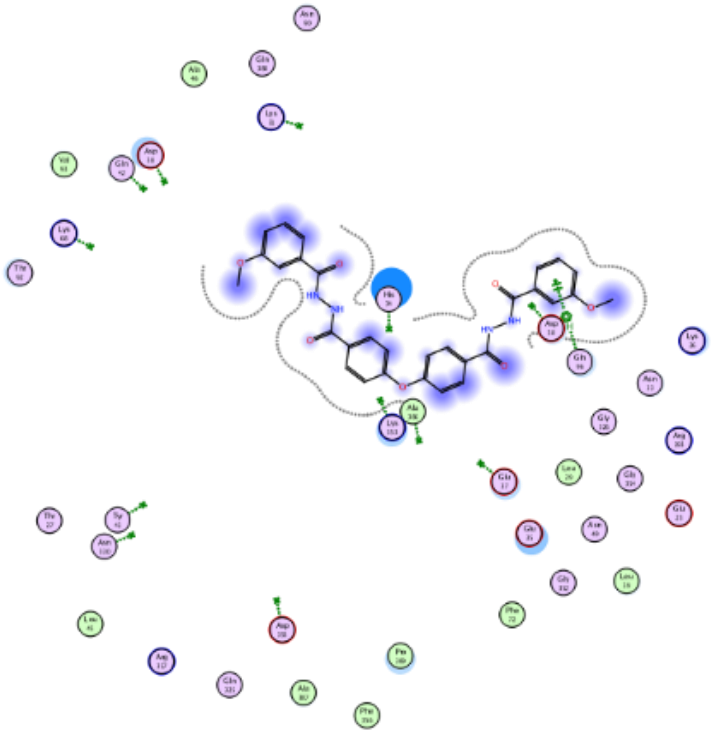
Table S1: Representation of “ligand interactions” of 18 conformers of ED-compound interacting in the potential site in ACE2

Conformer 1	Conformer 2
	
Conformer 3	Conformer 4
	

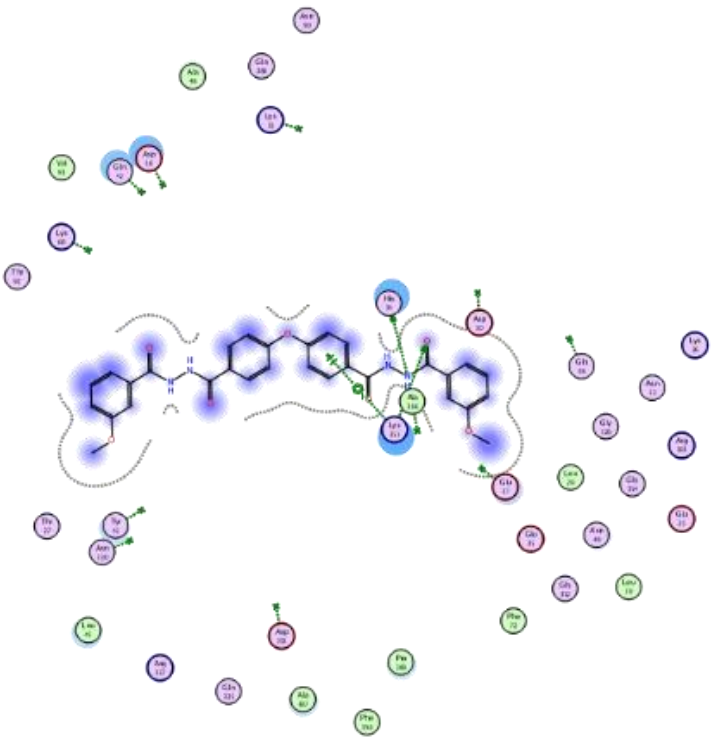
Conformer 5



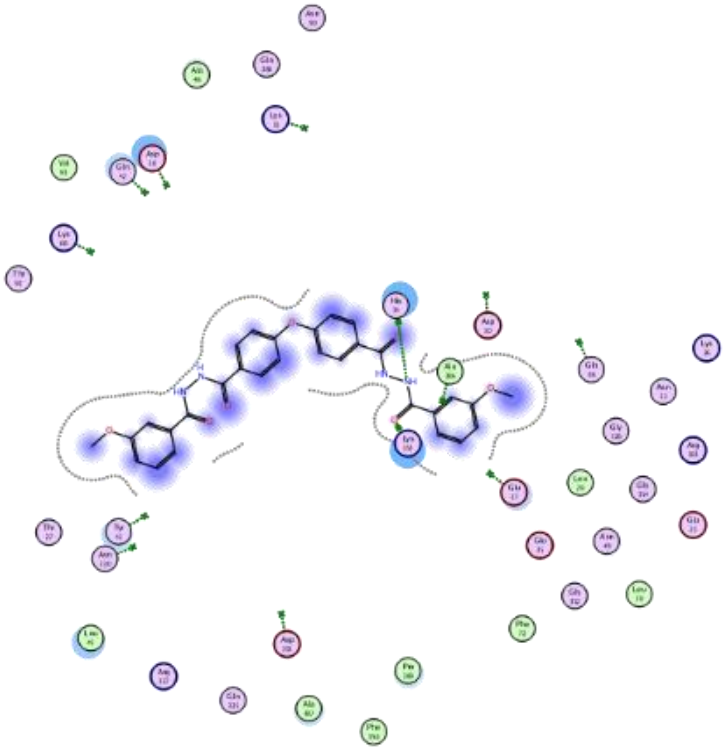
Conformer 6



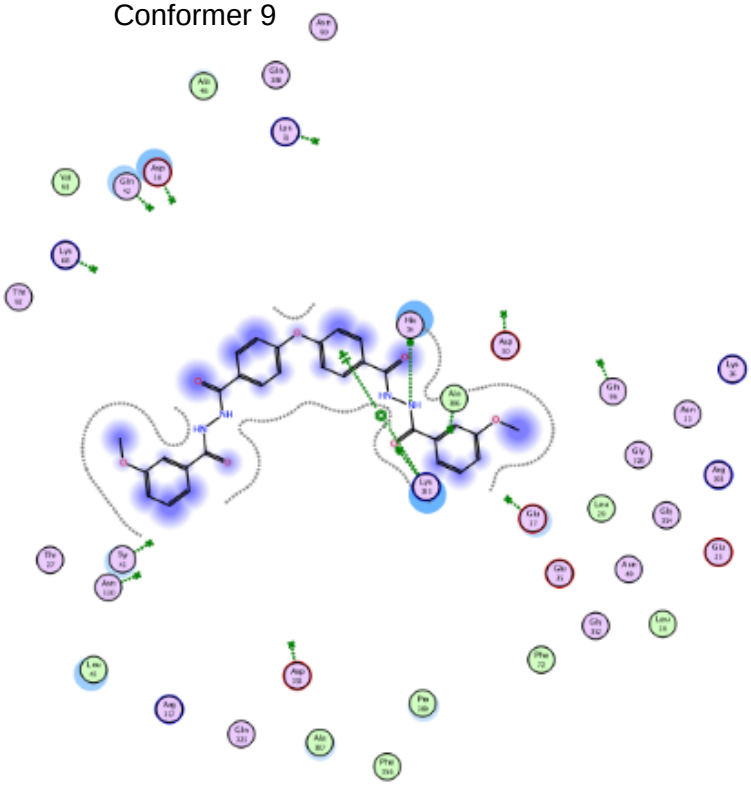
Conformer 7



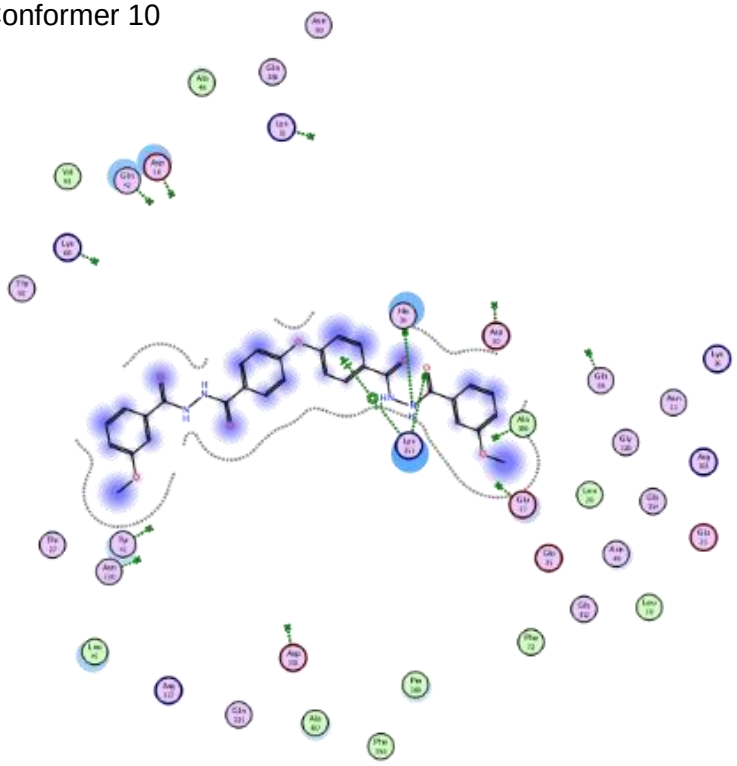
Conformer 8



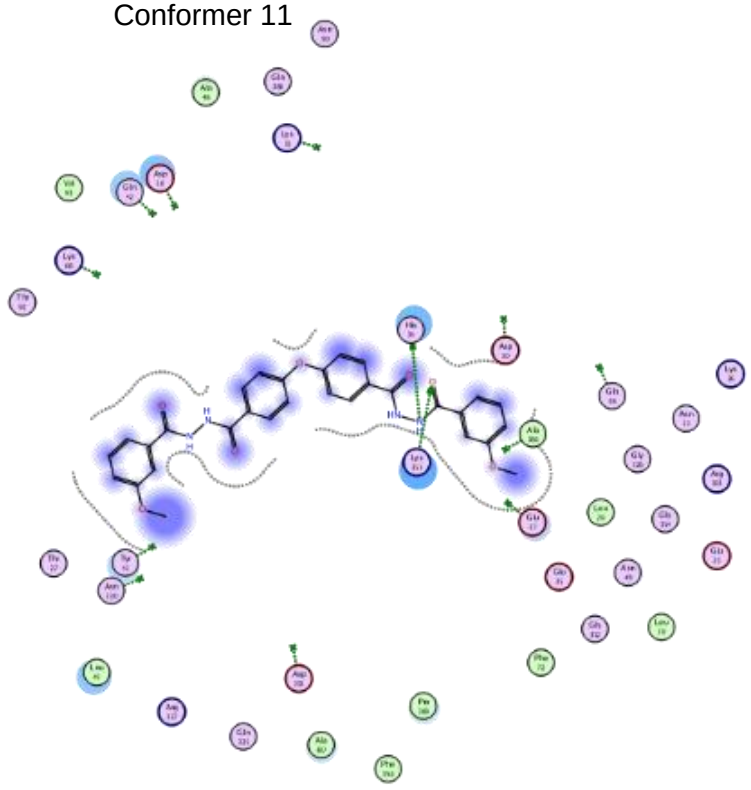
Conformer 9



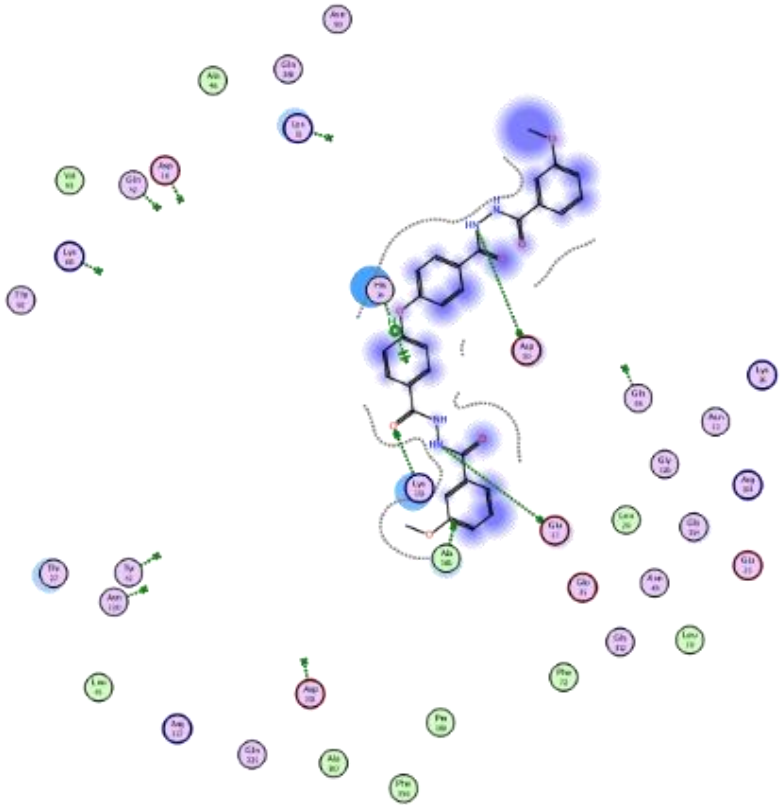
Conformer 10



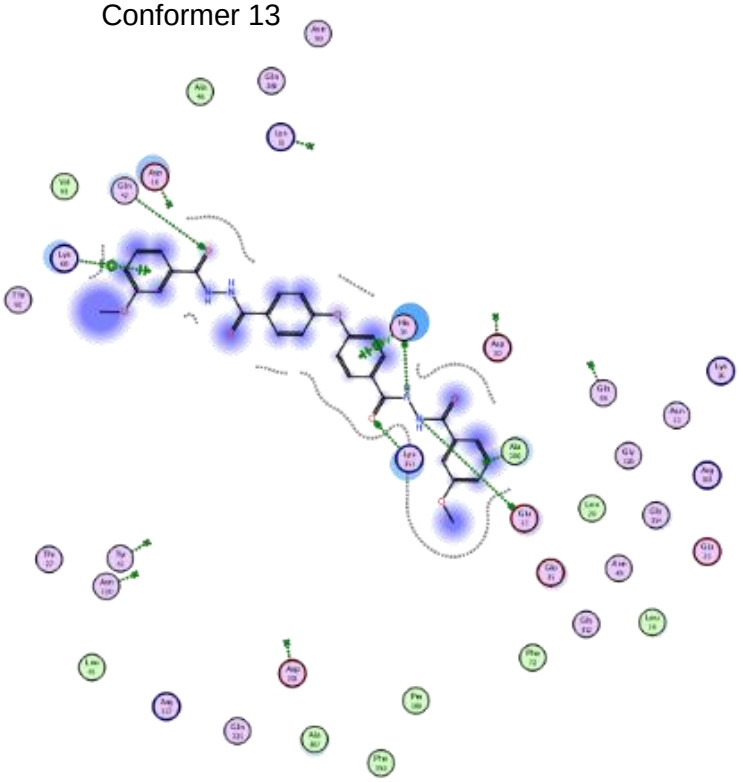
Conformer 11



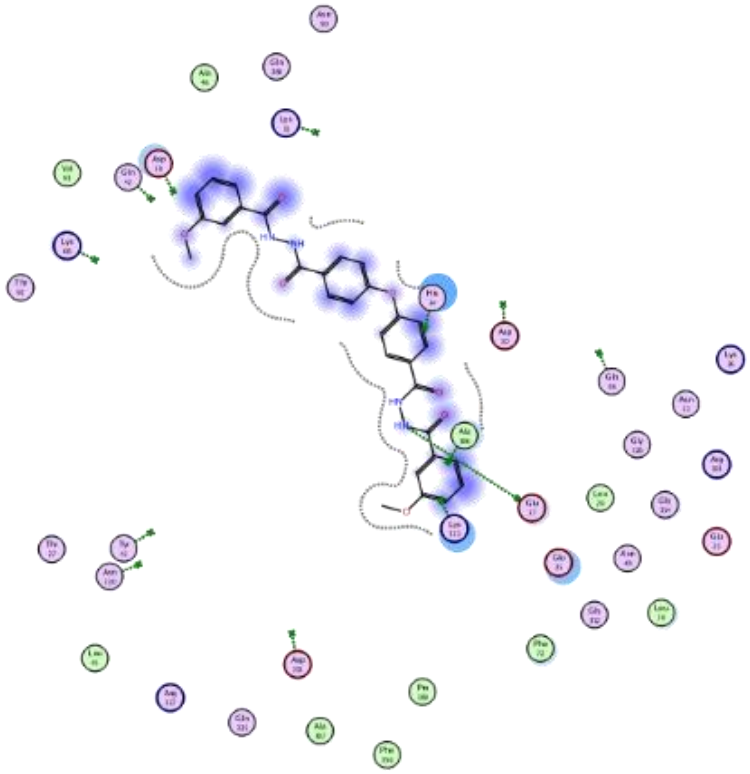
Conformer 12



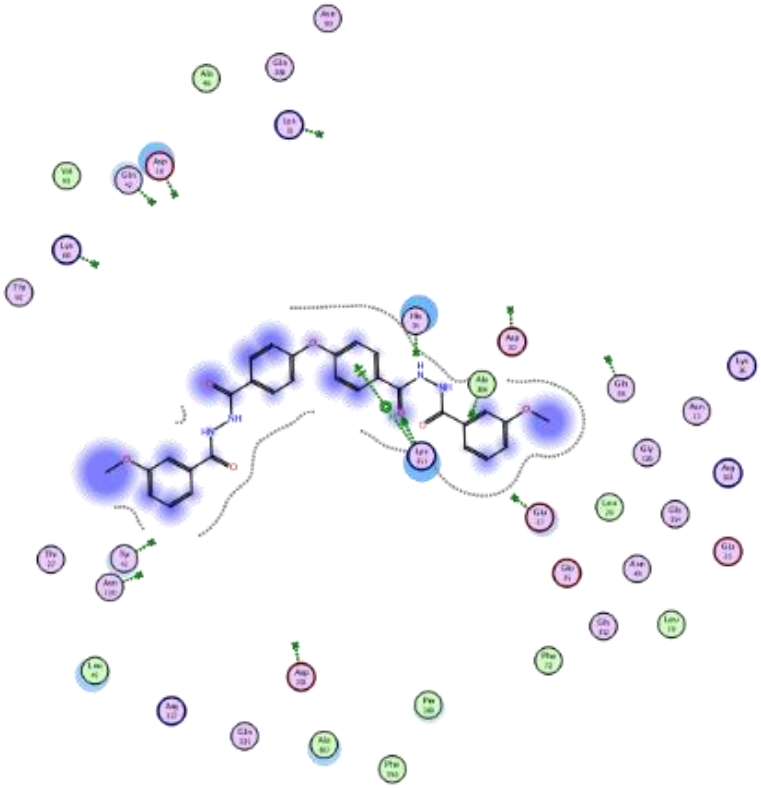
Conformer 13



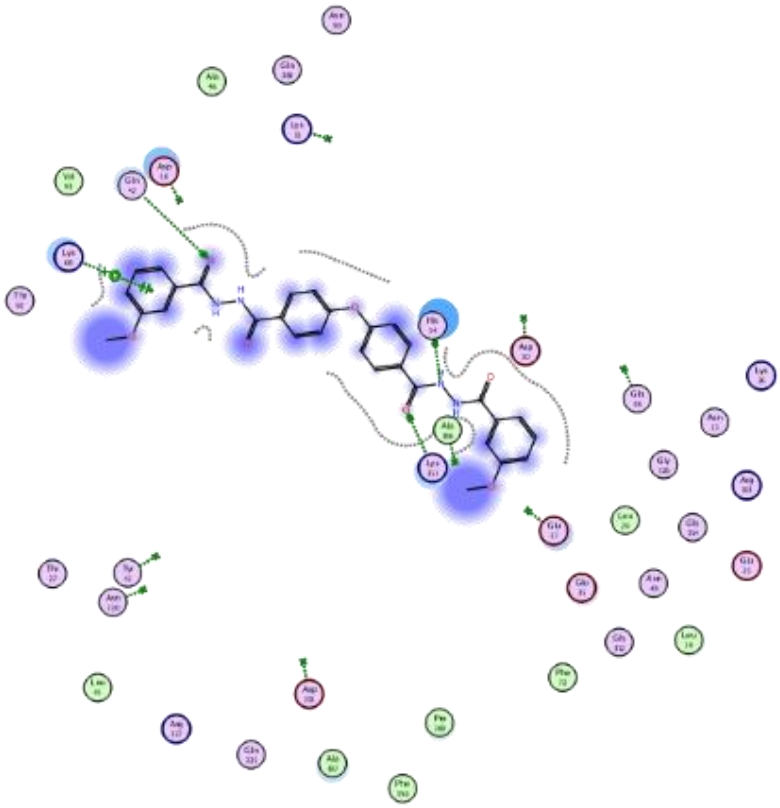
Conformer 14



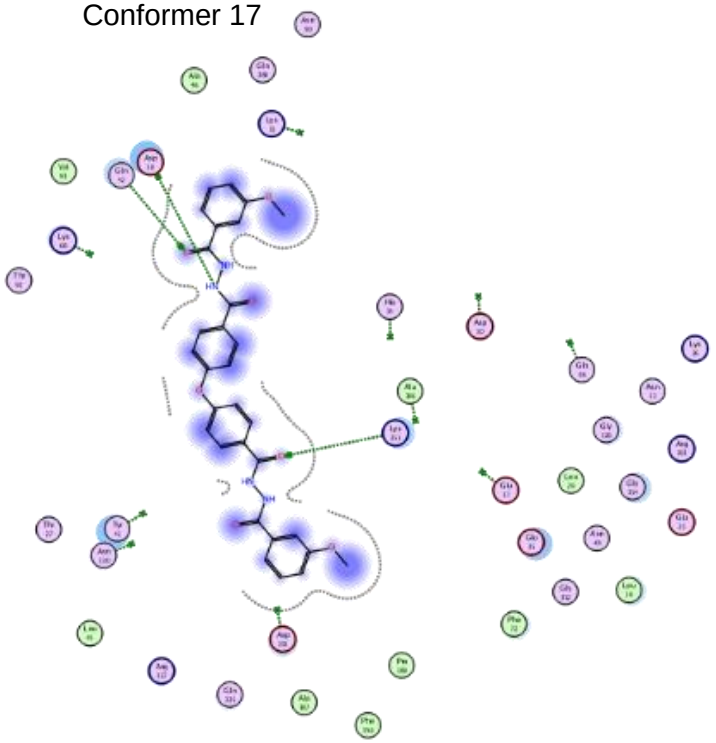
Conformer 15



Conformer 16



Conformer 17



Conformer 18

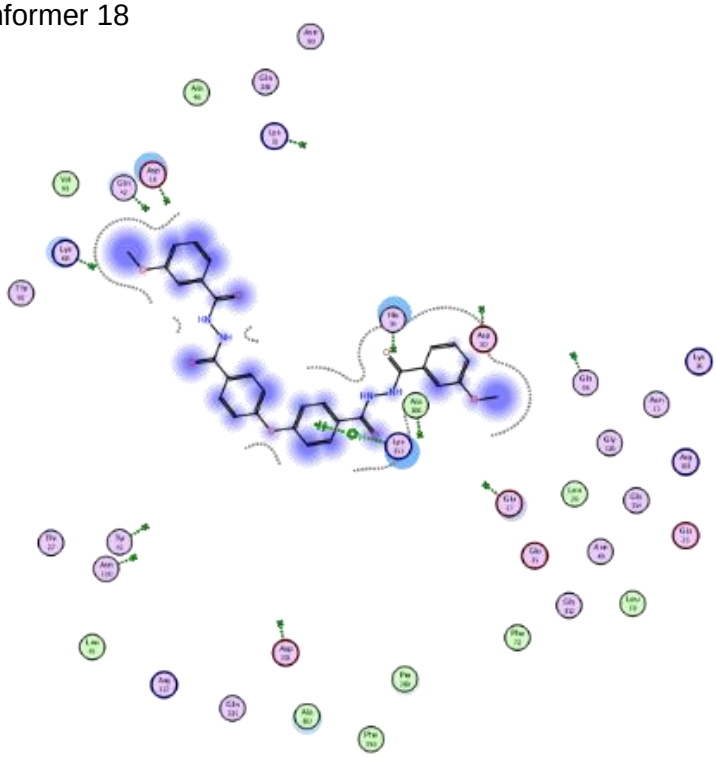


Table S2. Interaction report of each conformer of ED-compound. Number of conformer, Atom of compound, Amino acid in ACE2, Type of interaction and Energy.					
Conformer	Ligand	Amino acid in ACE2		Interaction	E (kcal/mol)
1	N	His	34	H-donor	-4.1
	O	**Lys**	**353**	H-acceptor	-6.5
	O	Tyr	41	H-acceptor	-1.2
2	N	Asp	355	H-donor	-3.0
	6-ring	Asn	330	pi-H	-1.8
3	N	Glu	37	H-donor	-0.8
4	N	Glu	37	H-donor	-2.3
	N	His	34	H-donor	-1.0
	O	Lys	353	H-acceptor	-4.5
	6-ring	Lys	31	pi-H	-0.6
5	N	Asp	30	H-donor	-7.4
	N	Ala	386	H-donor	-2.2
6	6-ring	Gln	96	pi-H	-0.6
7	N	His	34	H-donor	-2.4
	O	Lys	353	H-acceptor	-4.9
	6-ring	Lys	353	pi-H	-0.9
8	N	His	34	H-donor	-2.8
	O	Lys	353	H-acceptor	-10.2
9	N	His	34	H-donor	-2.5
	O	Lys	353	H-acceptor	-10.2
	6-ring	Lys	353	pi-H	-1.1
10	N	His	34	H-donor	-2.0
	O	Lys	353	H-acceptor	-9.5
	6-ring	Lys	353	pi-H	-0.6
11	N	His	34	H-donor	-1.8
	O	Lys	353	H-acceptor	-9.5
12	N	Glu	37	H-donor	-0.7
	N	Asp	30	H-donor	-6.3
	O	Lys	353	H-acceptor	-5.9
	6-ring	His	34	pi-H	-0.8
13	N	Glu	37	H-donor	-2.8
	N	His	34	H-donor	-2.4
	O	Gln	42	H-acceptor	-1.1
	O	Lys	353	H-acceptor	-8.1
	6-ring	His	34	pi-H	-1.0
	6-ring	Lys	68	pi-cation	-3.7
14	N	Glu	37	H-donor	-1.2
15	O	Lys	353	H-acceptor	-1.2
	6-ring	Lys	353	pi-H	-0.7
16	N	His	34	H-donor	-2.6
	O	Gln	42	H-acceptor	-0.7

	O	**Lys**	**353**	H-acceptor	-12.7
	6-ring	Lys	68	pi-cation	-3.3
17	N	Asp	38	H-donor	-0.9
	O	Gln	42	H-acceptor	-1.4
	O	**Lys**	**353**	H-acceptor	-0.7
18	6-ring	**Lys**	**353**	pi-H	-1.4

Table S3. ED-compound. PubChem CID, ID, Canonical Smile, Interaction with residues in ACE2, Number of conformers used, $\Delta G_{binding}$ average (kcal/mol-1) with standard deviation (SD), Reported theoretical toxicity/Ames test and LD50 [11].

PubChem CID, ID Chembridge Corp.	Canonical Smile	Interaction with residues in ACE2 (Table S1 – S20)	Number of conformers	Average of $\Delta G_{binding}$ and SD	Toxicity Model Report from ProTox-II server / PreADMET Ames test	Predicted LD50 (mg/kg)
2953854, 7781334	COC1=CC=CC(=C1)C(=O)NNC(=O)C2=CC=C(C=C2)OC3=CC=C(C=C3)C(=O)NNC(=O)C4=CC(=CC=C4)OC	Asp30, His34, Glu37, Asp38, Tyr41, Gln42, Lys68, Asn330, **Lys353**, Asp355 and Ala386	18	-5.87 ± 0.49	Aryl hydrocarbon Receptor (AhR) 53 % / Non mutagen	575