

*Communication*

# **Conservation and Enhanced Binding of SARS-CoV-2 Omicron Spike Protein to Coreceptor Neuropilin-1 Predicted by Docking Analysis**

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**Table S1.** Amino acid interaction analysis of docking complex between Nrp1 and S protein (CendR) of Wuhan and Omicron variant.

Nrp1_spolybasic (Wuhan)							
Name	Distance	Category	Types	From	From chemistry	To	To chemistry
A:ARG39:NH1 - A:GLU541:OE1	2.848 44	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG39:NH1	H-Donor	A:GLU541:OE1	H-Acceptor
A:ARG42:NH1 - A:GLU550:OE1	2.472 42	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG42:NH1	H-Donor	A:GLU550:OE1	H-Acceptor
A:ARG39:NH2 - A:GLU550:OE2	4.599 4	Electrostatic	Attractive Charge	A:ARG39:NH2	Positive	A:GLU550:OE2	Negative
A:ARG40:NH2 - A:GLU541:OE2	3.785 55	Electrostatic	Attractive Charge	A:ARG40:NH2	Positive	A:GLU541:OE2	Negative
A:THR35:N - A:CYS275:SG	3.393 95	Hydrogen Bond	Conventional Hydrogen Bond	A:THR35:N	H-Donor	A:CYS275:SG	H-Acceptor
A:ARG39:NH2 - A:GLY542:O	3.119 31	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG39:NH2	H-Donor	A:GLY542:O	H-Acceptor
A:ALA41:N - A:PRO38:O	3.103 68	Hydrogen Bond	Conventional Hydrogen Bond	A:ALA41:N	H-Donor	A:PRO38:O	H-Acceptor
A:ARG42:N - A:PRO38:O	3.064 75	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG42:N	H-Donor	A:PRO38:O	H-Acceptor
A:PRO398:CD - A:ARG42:O	3.532 23	Hydrogen Bond	Carbon Hydrogen Bond	A:PRO398:CD	H-Donor	A:ARG42:O	H-Acceptor
A:PRO38:CD - A:THR553:OG1	2.734 66	Hydrogen Bond	Carbon Hydrogen Bond	A:PRO38:CD	H-Donor	A:THR553:OG1	H-Acceptor
A:ARG42:CD - A:THR35:O	3.186 32	Hydrogen Bond	Carbon Hydrogen Bond	A:ARG42:CD	H-Donor	A:THR35:O	H-Acceptor
A:ALA41 - A:PRO38	4.141 75	Hydrophobic	Alkyl	A:ALA41	Alkyl	A:PRO38	Alkyl
A:ARG42 - A:PRO398	4.300 74	Hydrophobic	Alkyl	A:ARG42	Alkyl	A:PRO398	Alkyl
Nrp1_spolybasic (Omicron)							
A:ARG45:NH2 - A:GLU550:OE1	3.180 58	Hydrogen Bond;Electrostatic	Salt Bridge	A:ARG45:NH2	H-Donor	A:GLU550:OE1	H-Acceptor
A:LYS41:NZ - A:GLU541:OE2	5.054 73	Electrostatic	Attractive Charge	A:LYS41:NZ	Positive	A:GLU541:OE2	Negative
A:ARG45:NH1 - A:GLU550:OE2	4.704 86	Electrostatic	Attractive Charge	A:ARG45:NH1	Positive	A:GLU550:OE2	Negative
A:ARG44:NH1 - A:CYS431:O	2.888 15	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG44:NH1	H-Donor	A:CYS431:O	H-Acceptor
A:ARG45:N - A:SER42:O	3.032 12	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG45:N	H-Donor	A:SER42:O	H-Acceptor
A:ARG45:NH2 - A:PRO398:O	2.807 79	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG45:NH2	H-Donor	A:PRO398:O	H-Acceptor
A:ARG45:CD - A:PRO398:O	3.435 62	Hydrogen Bond	Carbon Hydrogen Bond	A:ARG45:CD	H-Donor	A:PRO398:O	H-Acceptor
A:ARG44 - A:LEU551	4.586 83	Hydrophobic	Alkyl	A:ARG44	Alkyl	A:LEU551	Alkyl
A:ARG45 - A:PRO398	3.739 45	Hydrophobic	Alkyl	A:ARG45	Alkyl	A:PRO398	Alkyl
A:ALA46 - A:CYS275	4.509 89	Hydrophobic	Alkyl	A:ALA46	Alkyl	A:CYS275	Alkyl
A:ALA46 - A:PRO398	4.726 47	Hydrophobic	Alkyl	A:ALA46	Alkyl	A:PRO398	Alkyl
A:PHE335 - A:ARG44	5.131 31	Hydrophobic	Pi-Alkyl	A:PHE335	Pi-Orbitals	A:ARG44	Alkyl
A:PHE335 - A:ARG45	4.394 68	Hydrophobic	Pi-Alkyl	A:PHE335	Pi-Orbitals	A:ARG45	Alkyl
A:TYR429 - A:ARG44	4.300 1	Hydrophobic	Pi-Alkyl	A:TYR429	Pi-Orbitals	A:ARG44	Alkyl