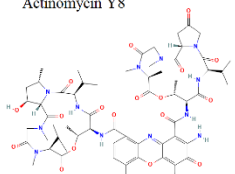


Appendix 1. Comparison of validation of predicted 3D models of variants of SARS-CoV-2 RBD with wild-type by different scores

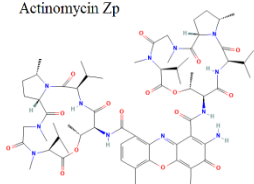
Protein	Ramachandran plot quality (%)				Verify3D (%)	ERRAT (%)
	Most favored	Additionally allowed	Generously allowed	Disallowed		
Wild-type	83.7	15.7	0.0	0.6	91.71	90.909
Alpha	83.6	15.8	0.0	0.6	91.71	87.500
Beta	83.7	15.7	0.0	0.6	92.23	87.500
Delta	83.7	15.7	0.0	0.6	92.23	90.909
Lambda	83.7	15.7	0.0	0.6	92.75	90.909
Omicron/BA.1	82.7	16.1	0.0	1.2	92.23	85.227
Omicron/BA.2	83.7	15.7	0.0	0.6	92.75	85.795

Appendix 2

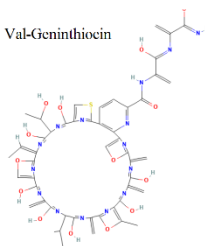
Actinomycin Y8



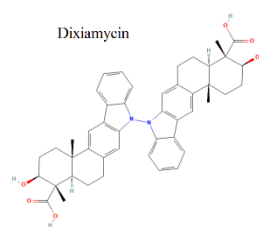
Actinomycin Zp



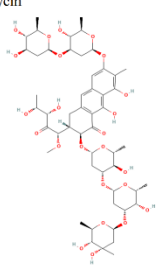
Val-Geninthiocin



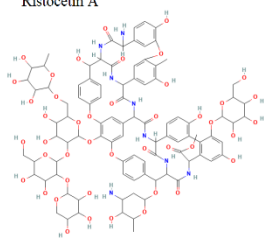
Dixiamycin



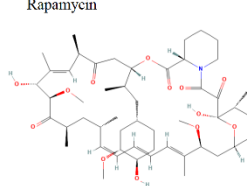
Plicamycin



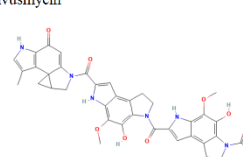
Ristocetin A



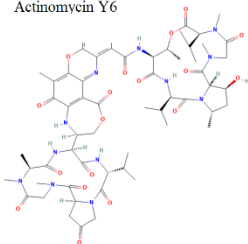
Rapamycin



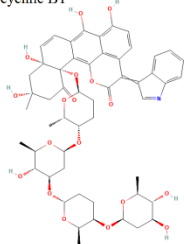
Gilvusmycin



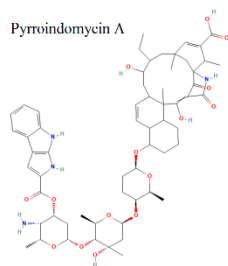
Actinomycin Y6



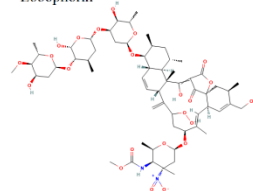
Langkocycline B1



Pyroindomycin A



Lobophorin



Appendix 3. Evaluation binding affinity and interaction summary of ‘Stambomycin B’ with wild-type and variants.

Protein	<u>Stambomycin B</u>			
	Binding affinity (Kcal/mol)	HB-AAs ^a	angle / Bond length	NH-AAs ^b
Wild-type	-11.60	Lys403	N—H—O = 48.25° / 2.85 Å	Tyr449
		Lys403		Gln493
		Glu484	N—H—N = 59.18° / 3.25 Å	Tyr453
		Ser494	O—H—O = 83.81° / 3.02 Å	Tyr505
		Thr500	O—H—O = 159.84° / 3.07 Å	
		Asn501	O—H—O = 59.46° / 2.67 Å	

			$\text{N—H—O} = 78.86^\circ /$ 2.86 \AA	
Alpha	-10.60	Gln493 Thr500 Gly502	$\text{N—H—O} = 154.58^\circ /$ 3.25 \AA $\text{O—H—O} = 115.28^\circ /$ 3.05 \AA $\text{N—H—O} = 19.78^\circ /$ 2.86 \AA	Val417 Leu455 Tyr449 Phe456 Thr500 Tyr501 Gly502 Tyr505

Beta	-12.00	Asp406	O—H—O =135.40°/ 2.84 Å	Lys403
		Asp406		Asn417
		Gln409	O—H—O =150.12°/ 2.91 Å	Tyr449
		Tyr453	N —H—O =78.34°/ 2.84 Å	Gln493
		Ser494	O—H—O = 91.06°/ 3.01 Å	
		Ser494	O—H—O = 75.77°/ 2.72 Å	
		Ser494	O—H—O = 40.33°/ 3.16 Å	
		Tyr501	O—H—O = 80.23°/ 3.00 Å	
			O—H—O = 68.45°/ 3.25 Å	
		Asp406	O—H—O = 147.09°/ 2.86 Å	Lys403

Delta	-12.47	Asp406	O—H—O = 103.01°/ 2.84 Å	Asn417
		Gln409	N—H—O = 124.06°/ 2.81 Å	Tyr449
		Tyr453		Gln493
		Ser494	O—H—O = 65.30°/ 3.00 Å	Asn501
		Ser494	O—H—O = 89.70°/ 2.86 Å	
		Ser494	O—H—O = 85.05°/ 2.94 Å	
			O—H—O = 85.05.33°/ 2.94 Å	
		Lys403	N—H—O = 117.19°/ 2.87 Å	Tyr449
		Lys403		Tyr453
		Glu484	N—H—N = 134.84°/ 3.29 Å	Gln493

Lambda	-11.64	Ser494	O—H—O =76.66°/ 3.05 Å	Tyr505
		Thr500	O—H—O =97.02°/ 3.09 Å	
		Asn501	O—H—O =102.34°/ 2.67 Å	
			N—H—O =85.93°/ 2.84 Å	
Omicron/B A.1	-12.56	Ser494	O—H—O =169.63°/ 2.88 Å	Lys403
		Thr500		Tyr449
		Tyr501	O—H—O =130.63°/ 3.02 Å	Arg493
			O—H—O =130.68°/ 3.02 Å	Ser496
				His505

Omicron/B A.2	-11.44	Gly485	O—H—O =79.46°/ 2.81 Å	Leu455
		Cys488	O—H—O =128.69°/ 2.83 Å	Ala484
		Arg493	N—H—O =53.9°/ 3.02 Å	Tyr489
		Gly502	N—H—O =104.10°/ 3.13 Å	Phe490
				His505
^a Hydrogen bonds forming Amino Acids, ^b Hydrophobic bonds forming Amino Acids,				