

Table S1. Docking scores for the RBD and hACE2 complexes.

	Delta wild type	501Y mutant	452L-484E mutant
Docking score (cal/mol)	-276.54	-341.94	-302.95
Ligand RMSD(Å)	0.69	0.48	1.45

RMSD, root-mean-square deviation; RBD, receptor-binding domain; hACE2, human angiotensin-converting enzyme 2.