Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Single point mutations can potentially enhance infectivity of SARS-CoV-2 revealed by in silico affinity maturation and SPR assay

Ting Xue,[a#] Weikun Wu,[b#] Ning Guo,[b] Chengyong Wu,[a] Jian Huang,[b] Lipeng Lai,[b]
Hong Liu,[a] Yalun Li,[a] Tianyuan Wang,[b*] and Yuxi Wang,[a*]

a Targeted Tracer Research and Development Laboratory, Precision Medicine Research Center, Department of Respiratory and Critical Care Medicine, West China Hospital, Sichuan University, Chengdu 610041, P.R. China
b XtalPi - AI Research Center (XARC), 9F, Tower A, Dongsheng Building, No.8, Zhongguancun East Road, Haidian District, Beijing 100083, P.R. China

[#]These authors contributed equally to this work.

Contents

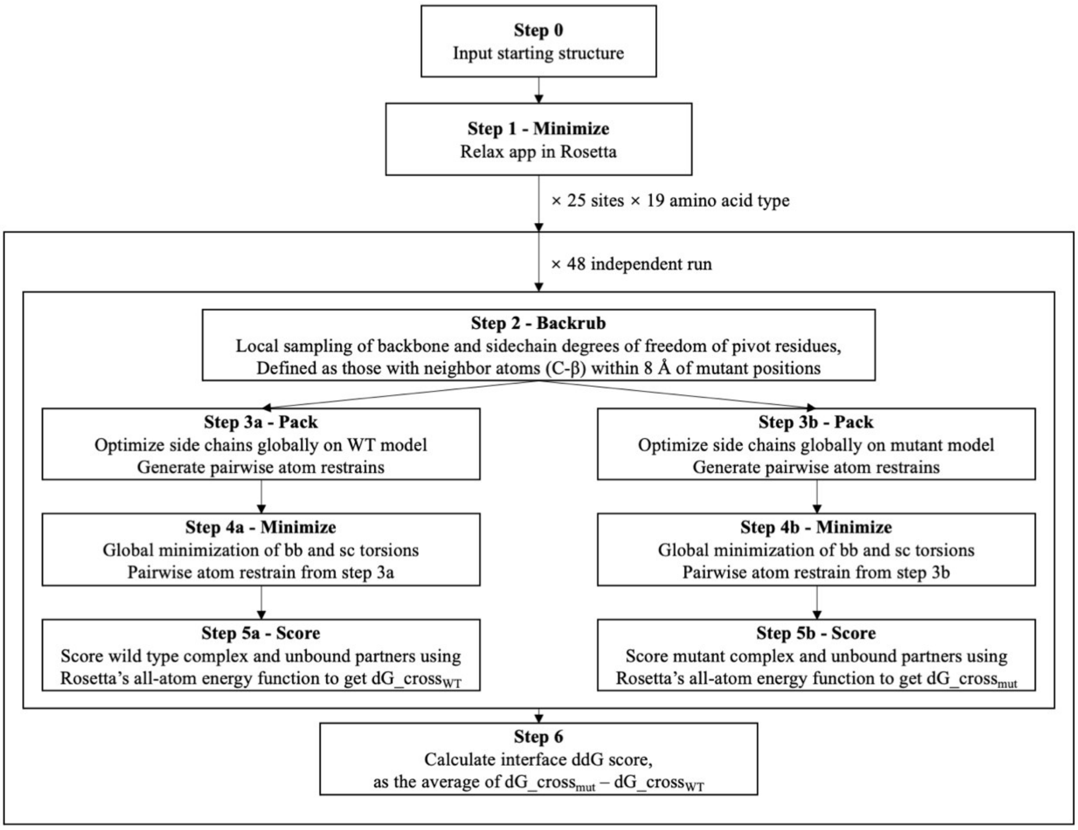

Figure S1. Schematic of the flex ddG protocol, modified from the flex ddG paper.

Table S1. List of the sample name on the SDS-PAGE figure corresponding to the mutants.

Sample name on the SDS-PAGE figure	Mutant
P101154-1	RBD-Q498W
P101154-2	RBD-Q498R
P101154-3	RBD-T500W
P101154-4	RBD-S477H
P101154-5	RBD-Y505W
P101154-6	RBD-T500R
P101154-7	RBD-N501V
P101154-8	RBD-Y489W
P101154-9	RBD-Q493M
P101154-10	RBD-L455A

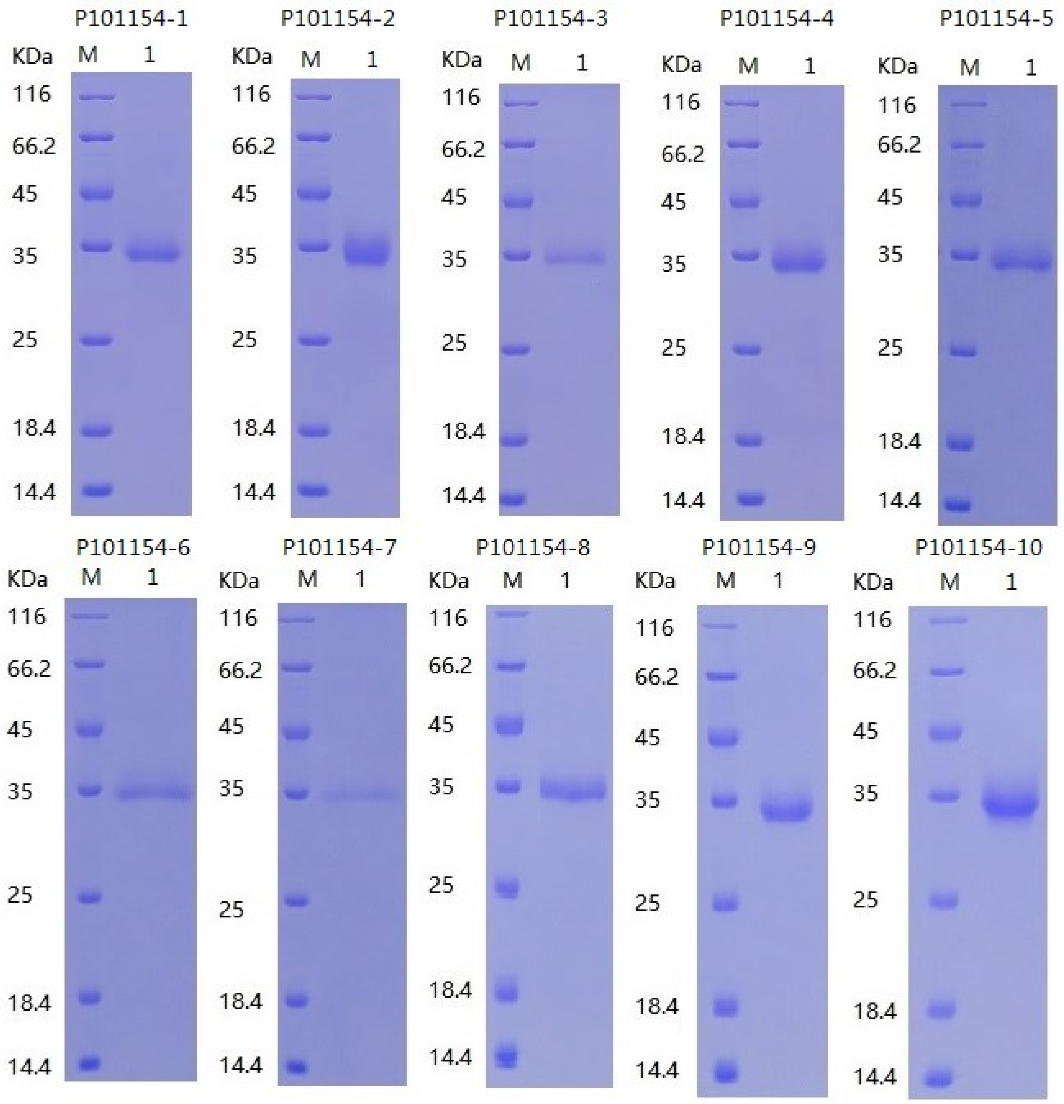

Figure S2. SDS-PAGE result of the 10 spike protein RBD mutants. M: Protein marker. 1: Corresponding protein sample. The sample name and related mutant is shown in Table S2.

Table S2. SPR result of RBD-WT and 10 mutants.

Sample name	Protein concentration (mg/mL)	Ka (1/(M*s))	Kd (1/s)	KD (M)
RBD-WT	0.25	3.6677E+04	9.048E-04	2.467E-8
RBD-Q498W	0.08	6.1757E+04	4.363E-04	7.065E-9
RBD-Q498R	0.35	9.3103E+04	1.081E-03	1.161E-8
RBD-T500W	0.06	1.4307E+04	3.117E-04	2.179E-8
RBD-S477H	0.19	7.3496E+04	1.021E-03	1.389E-8
RBD-Y505W	0.1	4.0716E+04	6.743E-04	1.656E-8
RBD-T500R	0.05	6.783E+03	8.253E-05	1.217E-8
RBD-N501V	0.05	1.623E+03	2.572E-04	1.585E-7
RBD-Y489W	0.1	1.5902E+04	6.189E-04	3.892E-8
RBD-Q493M	0.31	6.2167E+04	4.281E-04	6.886E-9
RBD-L455A	0.32	1.3389E+04	2.789E-04	2.083E-8

Ka: association (on) rate; Kd: dissociation (off) rate; KD: binding affinity constant