

Supplementary Information

Molecular Dynamics Studies of Disulfide Bonds for Enhancing the Stability of Serine Protease PB92

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Table S1 The results indicate that potential disulfide bond mutation sites exhibit superior stability compared to the wild-type screened by FoldX

| | Total energy (Kcal/mol) | Backbone Hbond (Kcal/mol) | Van der Waals (Kcal/mol) | Electrostatics (Kcal/mol) | Disulfide (Kcal/mol) |
|-------------|----------------------------|------------------------------|-----------------------------|------------------------------|-------------------------|
| Wild-Type | 337.426 | -97.900 | -271.310 | -3.39328 | / |
| V148C-M169C | 331.374 | -98.3861 | -268.946 | -3.24545 | -3.30125 |
| T247C-A266C | 329.512 | -98.7259 | -271.466 | -3.42761 | -3.13302 |
| G116C-V145C | 281.728 | -113.348 | -266.786 | -4.69662 | -3.50429 |
| A173C-G196C | 321.934 | -100.535 | -271.564 | -3.485 | -3.36904 |
| N121C-A222C | 329.054 | -97.4736 | -271.423 | -3.39926 | -4.70725 |
| A71C-A86C | 305.135 | -102.455 | -269.708 | -3.73751 | -3.03035 |
| G45C-Y89C | 327.384 | -99.0607 | -270.143 | -3.33747 | -3.77936 |
| V50C-S104C | 327.739 | -98.3102 | -270.721 | -3.4327 | -4.14667 |
| S48C-K92C | 323.534 | -97.4139 | -268.987 | -2.89956 | -3.57904 |
| F49C-Q107C | 325.15 | -99.6695 | -267.574 | -3.43363 | -4.16332 |
| T249C-L261C | 295.218 | -104.363 | -265.623 | -3.82926 | -2.70623 |
| G7C-V199C | 318.13 | -100.808 | -271.137 | -3.45575 | -5.26571 |
| T247C-A267C | 325.858 | -99.7812 | -271.257 | -3.46956 | -3.1533 |
| R44C-E87C | 321.129 | -98.7859 | -268.752 | -2.60212 | -3.86395 |
| Q200C-S210C | 331.675 | -97.8976 | -270.757 | -3.39315 | -2.61689 |