Table 1: MM/GBSA

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Peptides | VDW | ELE | GB | SA | Binding free energy of complex  (kcal/mol) |
| 1a\_G446V\_AMU | -92.33 | 95.4 | -34.39 | -12.07 | -43.4 |
| 1b\_G446V\_DK25 | -75.57 | -27.64 | 74.23 | -10.99 | -39.96 |
| 1c\_G446V\_ODO | -55.3 | -53.15 | 72.54 | -7.69 | -43.59 |
| 2a\_L452R\_AMU | -92.48 | 154.69 | -92.33 | -11.93 | -42.06 |
| 2b\_L452R\_DK25 | -77.6 | 25.85 | 23.41 | -11.47 | -39.81 |
| 2c\_L452R\_PSE | -98.3 | 109.61 | -53.08 | -12.52 | -54.29 |
| 3a\_Y453F\_AMU | -89.63 | 84.5 | -27 | -11.51 | -43.63 |
| 3b\_Y453F\_DK25 | -70.76 | 12.27 | 37.38 | -9.9 | -31.01 |
| 3c\_Y453F\_LIV | -68.52 | -26.73 | 69.9 | -9.45 | -34.8 |
| 4a\_S477G\_AMU | -90.78 | 60.08 | -4.46 | -11.54 | -46.69 |
| 4b\_S477G\_BOM | -60.4 | -77.41 | 105.4 | -7.44 | -39.85 |
| 4c\_S477G\_XPF | -102.58 | -14.46 | 87.87 | -11.8 | -40.96 |
| 5a\_S477N\_OPI | -70.15 | 43.52 | -9.56 | -9.54 | -45.73 |
| 5b\_S477N\_AMU | -94.91 | 60.56 | -1.49 | -12.22 | -48.07 |
| 5c\_S477N\_DK25 | -80.87 | 20.8 | 42.05 | -10.81 | -28.83 |
| 6a\_S477R\_BOM | -62.79 | -43.78 | 89.29 | -8.82 | -26.1 |
| 6b\_S477R\_GRN | -74.5 | 108.13 | -44.13 | -9.91 | -20.41 |
| 6c\_S477R\_SCN | -68.13 | -107.76 | 153.72 | -9.58 | -31.75 |
| 7a\_E484K\_ASC | -69.77 | 232.56 | -194.61 | -9.11 | -40.94 |
| 7b\_E484K\_DK25 | -74.42 | 24.75 | 21.43 | -11.02 | -39.26 |
| 7c\_E484K\_PSE | -82.92 | 171.42 | -110.82 | -11.01 | -33.33 |
| 8a\_E484A\_DK25 | -74.18 | -9.11 | 47.19 | -10.67 | -46.77 |
| 8b\_E484A\_SCN | -52 | 43.16 | -3.38 | -7.17 | -19.4 |
| 8C\_E484A\_UPN | -60.24 | -128.04 | 155.81 | -7.92 | -40.38 |
| 9a\_E484D\_AMU | -95.15 | 87.12 | -21.57 | -12.19 | -41.79 |
| 9b\_E484D\_DK25 | -74.46 | -39.69 | 77.47 | -10.82 | -47.49 |
| 10a\_E484G\_AMU | -94.16 | 194.49 | -128.7 | -11.39 | -39.77 |
| 10b\_E484G\_PBV | -68.63 | 139.53 | -99.96 | -8.44 | -37.5 |
| 10c\_E484G\_PDS | -95.79 | 208.11 | -148.44 | -10.9 | -47.03 |
| 11a\_F490S\_AML | -64.05 | 179.05 | -132.95 | -7.98 | -25.93 |
| 11b\_F490S\_LIV | -63.43 | -48.78 | 78.17 | -9.28 | -43.31 |
| 11c\_F490S\_ODO | -70.23 | 19.56 | 33.19 | -9.97 | -27.45 |
| 12a\_N501Y\_BOM | -66.62 | -72.58 | 107.1 | -8.13 | -40.24 |
| 12b\_N501Y\_PRP | -83.59 | 103.69 | -50.07 | -9.65 | -39.62 |
| 12c\_N501Y\_UPN | -57.07 | -104.58 | 135.93 | -7.6 | -33.33 |
| 12d\_N501Y\_XNP | -85.95 | 9.62 | 31.65 | -11.22 | -55.9 |