Table 5. Binding free energy and energy components calculated by MM/GBSA (kcal/mol)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **RELA** | **IL-6** | **VEGFA** | **MMP9** |
| **∆EvdW**  | -34.79 ± 2.30 | -48.91±1.84 | -29.84±1.45 | -41.13±2.47 |
| **∆Eelec** | -11.59 ± 6.18 | -13.89±1.82 | -46.99±7.56 | -11.77±6.01 |
| **∆GGB** | 27.40 ± 5.81 | 32.05±1.40 | 61.36±7.71 | 33.98±5.63 |
| **∆GSA** | -4.09 ± 0.22 | -6.96±0.20 | -5.08±0.17 | -5.44±0.32 |
| **∆Gbind** | -23.06 ± 1.69 | -37.71±2.66 | -20.55±1.39 | -24.36±1.37 |

*∆EvdW: van der Waals energy*

*∆Eelec: electrostatic energy*

*∆GGB: electrostatic contribution to the solvation*

*∆GSA: non-polar contribution to the solvation*

*∆Gbind: binding free energy*