|  |  |  |
| --- | --- | --- |
| **Energy contributions** | **TNF-Shikimic acid** | **IL-6-Shikimic acid** |
| Δ*VDWAALS* | -17.23±0.35 | -23.72±0.11 |
| Δ*Eelec* | -45.93±0.90 | -10.83±2.83 |
| Δ*EGB* | 45.03±0.49 | 19.62±0.53 |
| Δ*Esurf* | -3.65±0.00 | -3.73±0.01 |
| Δ*Ggas* | -63.17±0.97 | -34.56±2.83 |
| Δ*Gsolvation* | 41.38±0.49 | 15.89±0.53 |
| Δ*GBind* | -21.79±1.08 | -18.67±2.88 |

Table 1. Binding free energy analysis of TNF-Shikimic acid and IL-6-Shikimic acid complexes (kcal/mol)