**Table 3.** MM-PBSA binding free energies of FabH with compounds **E9** and **E10** between 80ns and 100 ns.

|  |  |  |
| --- | --- | --- |
|  | **Enzyme-ligand complexes** | |
| **Parameters**  (Energy) | **FabH & E9**  (kJ/mol) | **FabH & E10**  (kJ/mol) |
| Van der Waals | -207.305±12.271 | -272.200±10.109 |
| Electrostatic | 3.695±3.356 | 1.563±2.200 |
| Polar solvation | 41.219±13.297 | 45.524±6.006 |
| SASA | -18.603 0.999 | -20.690± 0.835 |
| Binding free | **-180.993±15.364** | **-245.803±10.893** |