**Table 4:** Molecular Interaction profile of Compound 9 with EGFR Kinase domain during MD simulation:

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| S.No | Drug Target | Compound Name | Molecular interactions compound 9 with active site of EGFR kinase domain | | | | |
| **H-Bonds** | **Hydrophobic interactions** | **Ionic bonds** | **Water bridging residues** | **Pi-Pi stacking** |
|  | EGFR Kinase domain | Compound 9 | MET769 | LEU692; LEU694; SER696; PHE699; VAL702; ALA719; LYS721; MET742;  LEU768; PHE771; CYS773; ASP776; ARG817; LEU820 | None | LYS704; LYS721; MET742; THR766; GLN767; PRO770; GLY772; ASP831. | PHE699 |