**Table 2**. Glide XP molecular docking, Prime binding free energy and protein-ligand interactions results performed against bacterial (FabH) and fungal (CYP51) target enzymes

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Target enzymes | Comp. | XP GScore | MMGBSA dG Bind | Protein-ligand interactions |
| FabH  (PDB ID: 3IL5) | **E6** | -8.75 | -60.11 | **Asn253** (2.50Å), **Asn280** (2.80Å, 1.96Å), Asn280, Phe312, Ile223, Ala227, Ala252, Ile223, Ala252 |
| **E9** | -8.50 | -65.52 | **Ala252** (2,06Å), Gly313, Phe312, Cys117, Leu194, His250, Arg221, Ala252, Ile223, Ala227, Ala252 |
| **E10** | -7.90 | -60.64 | Cys117, His250, Phe224, Arg221, Ile223, Ala252, Ile256, Leu194, Ile223, Ala252 |
| **E13** | -8.33 | -56.69 | **Gly220** (2.51Å), **Ala252** (1.97Å), Met218, Phe312, Ala252, Ile223, Ala227, Ala252 |
| **E16** | -7.51 | -61.75 | **Gly220** (2.42Å), **Ala252** (2.24Å), Ala252, Met218, Phe312, Ile223, Ile223, Ala227, Ala252 |
| CYP51  (PDB ID: 5TZ1) | **E6** | -7.97 | -47.97 | Phe380, Phe233, Leu376, Leu376, Ile131, Hem601 |
| **E16** | -7.07 | -47.94 | **Met508** (3.69Å), Tyr118, Tyr118, His377, Pro230, Pro230, Met508, Leu121, Leu376, Met508, Leu376, Met508 |

FabH: Beta-ketoacyl-acyl carrier protein synthase III (PDB ID: 3IL5), CYP51: Sterol 14-alpha demethylase, XP Gscore (kcal/mol): Extra Precision Glide Score, MMGBSA dG Bind (kcal/mol): Molecular Mechanics Generalized Born Surface Area total binding energy