

## Supplementary material:

**Table 1:** IDH structural data

| Oragnism                   | DOPE score  | Z-score | Procheck Data |
|----------------------------|-------------|---------|---------------|
| <i>S. aureus</i> IDH       | -30911.646  | 8.24    | 91.3%         |
| <i>H. pylori</i> IDH       | -2848.9853  | 9.13    | 91.6%         |
| <i>M. tuberculosis</i> IDH | -89122.0312 | 11.92   | 93.8%         |

**Table 2:** Molecular docking interaction of isocitrate with the human and *S. aureus* IDH

| IDH              | Docking score (K.cal/mol) | No. of H-bonds | Interacting active site Residues | H-bond Length (Å) |
|------------------|---------------------------|----------------|----------------------------------|-------------------|
| <b>Human</b>     | -11.6169                  | 4              | D275                             | 2.7               |
|                  |                           |                | V276                             | 2.3               |
|                  |                           |                | V276                             | 2.5               |
|                  |                           |                | V276                             | 2.8               |
| <i>S. aureus</i> | -10.973                   | 4              | R20                              | 2.4               |
|                  |                           |                | D187                             | 2.3               |
|                  |                           |                | D187                             | 3.0               |
|                  |                           |                | N207                             | 2.2               |