

Table S1. The binding energy of interacted residues of receptors proteins of *M. tuberculosis* with diverse phytochemicals.

| Interactions with 3zxr | Binding Energy (kcal/mol) |
|------------------------------------|----------------------------------|
| Aloin | -6.28 |
| ISN | -5.424 |
| Oleanolic acid | -5.048 |
| Octyl- β -d- Glucopyranoside | -3.122 |
| Alliin | -2.421 |
| Phytol | -1.942 |
| EMB | -0.938 |
| Interactions with 3pty | Binding Energy (kcal/mol) |
| Aloin | -6.89 |
| ISN | -6.375 |
| Oleanolic acid | -4.27 |
| Octyl- β -d- Glucopyranoside | -4.462 |
| Alliin | -5.382 |
| Phytol | -1.113 |
| EMB | -2.963 |
| Interactions with 4ow8 | Binding Energy (kcal/mol) |
| Aloin | -5.209 |
| ISN | -5.91 |
| oleanolic acid | -3.628 |
| Octyl- β -d- Glucopyranoside | -4.395 |
| Alliin | -4.959 |
| Phytol | -1.316 |
| EMB | -2.66 |