**Table S1.** Molecular interactions of Stigmasterol, β-sitosterol, Chloroquine, Pyrimethamine and NADH with *pf*LDH

|  |  |  |
| --- | --- | --- |
| **Compound name** | **Compound ID** | **Interactions** |
|  |  | **H-Bond** | **Hydrophobic**  |
| Stigmasterol | 5280794 | Asp53 | Gly27, Ser28, Gly29, Met30, Ile31, Ile54, Val55, Met58, Thr97, Ala98, Gly99, Phe100, Thr101, Trp107, Arg109, Val138, Thr139, Asn140, Leu163, Leu167, Arg171, His195, Ala236, Val240, Ser245, Pro246, Tyr247, Pro250  |
| β-Sitosterol | 222284 | Asp53 | Gly27, Ser28, Gly29, Met30, Ile31, Ile54, Val55, Met58, Thr97, Ala98, Gly99, Phe100, Thr101, Trp107, Arg109, Val138, Thr139, Asn140, Val142, Leu163, Gly164, Leu167, Arg171, His195, Ala236, Pro246, Tyr247, Por250 |
| Chloroquine | 2719 | Thr97 | Gly29, Met30, Ile31, Ala98, Gly99, Phe100, Thr101, Arg109, Val138, Thr139, Asn140, Val142, Leu163, Leu167, Arg171, His195, Ser245, Pro246, Tyr246, Pro250 |
| Pyrimethamine | 4933 | Val138 | Met30, Ile31, Thr97, Gly99, Thr101, Trp107, Thr139, Asn140, Leu163, Leu167, Arg171, His197, Ala236, Tyr247, Ser245, Pro246, Pro250 |
| NADH (Co-crystallized ligand) | 439153 | Gly29, Met30, Ile31, Asp53, Phe100, Asn140, His195 | Gly27, Ser28, Gly32, Val55, Ile54, Met58, Thr97, Ala98, Gly99, Thr101, Ile119, Ile123, Val138, Thr139, Leu163, Leu167, Arg171, Pro246, Tyr247, Pro250 |