# Supporting information

# for

# Ensemble-based virtual screening of *Mycobacterium tuberculosis* ClpC1 inhibitors

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## Additional results data

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**Figure S1:** Ramachandran plot for *Mtb* ClpC1-NTD Model 1 generated from PROCHECK. The plot is displaying 100% amino acid residues located in the favourable regions.

**Table S1:** Search criteria used to extract ligands from the Super Natural II database.

|  |  |
| --- | --- |
| Criteria | Value |
| Molecular weight (Dalton) | 160 – 460 |
| logP | 2 – 4 |
| H-bond acceptors | 2 – 9 |
| H-bond donors | 2 – 4 |
| Toxicity class | Non-toxic |

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**Figure S2:** Generated graphs for protein MD simulation results. The (A) potential energy curve during minimisation, (B) temperature, (C) pressure, and (D) total energy plots produced for MD simulation analysis. The temperature, pressure, and total energy plots showed a stable trend over 100,000 ps MD simulation.



**Figure S3:** Generated graphs for protein-ligand complex MD simulation results. The (A) potential energy curve during minimisation, (B) temperature, (C) pressure, and (D) total energy plots produced for MD simulation analysis. The temperature, pressure, and total energy plots showed a stable trend over 100,000 ps MD simulation.

**Table S2:** The physicochemical properties for compounds NP132 and rufomycin I.

|  |  |  |
| --- | --- | --- |
|  | Compound | |
| Characteristics: | NP132 | Rufomycin I |
| Database ID | SN00055391 (Super Natural II) | 76871757 (PubChem) |
| Molecular weight (Dalton) | 386.16 | 1012.20 |
| logP | 2.0079 | 5.1774 |
| H-bond acceptors | 5 | 10 |
| H-bond donors | 2 | 6 |
| Toxicity class | Non-toxic | Slightly toxic |
| IUPAC name | 1-[3-(7-hydroxy-4,8-dimethyl-2-oxochromen-3-yl)propanamido]cyclohexane-1-carboxylate | (3S,6S,9S,12S,15S,21S)-15-[(E)-but-2-enyl]-6-[(4-hydroxy-3-nitrophenyl)methyl]-1,3,10-trimethyl-12-[[1-(2-methylbut-3-en-2-yl)indol-3-yl]methyl]-9,18,21-tris(2-methylpropyl)-1,4,7,10,13,16,19-heptazacyclohenicosane-2,5,8,11,14,17,20-heptone |
| Molecular formula | C21H24NO6 | C54H77N9O10 |