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Insights into anti-tuberculosis activity of partially purified bioactive fraction from *Vitex negundo* L. petroleum ether extracts against *Mycobacterium smegmatis* - An *in vitro* and *in silico* approach

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Supplementary Data

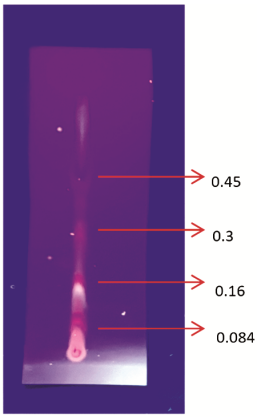

Fig. S1 — TLC fingerprint of petroleum ether extract crude of *Vitex negundo*

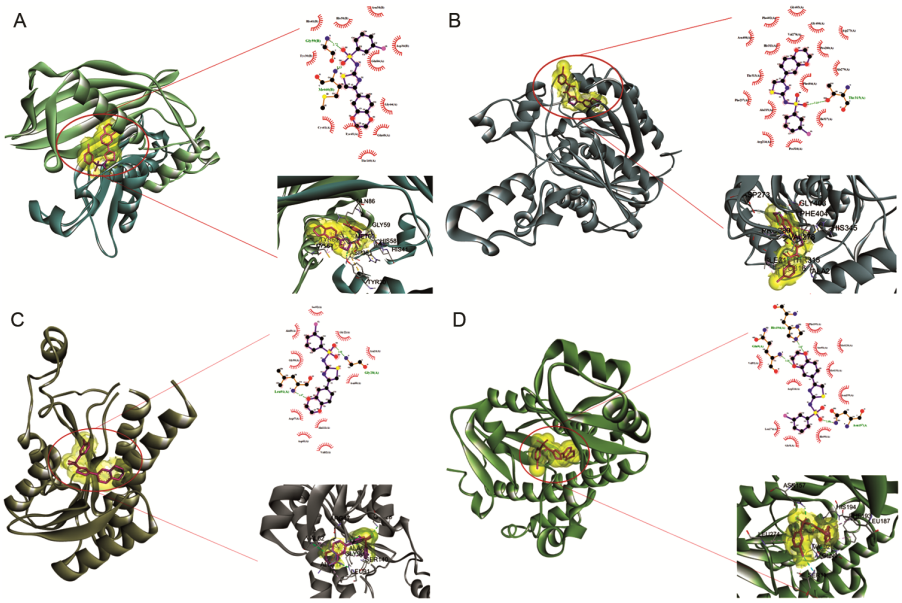

Fig. S2 — (A) HadAB; (B) KasA; (C) MabA; and (D) FabD protein interaction with Hit 3 compound

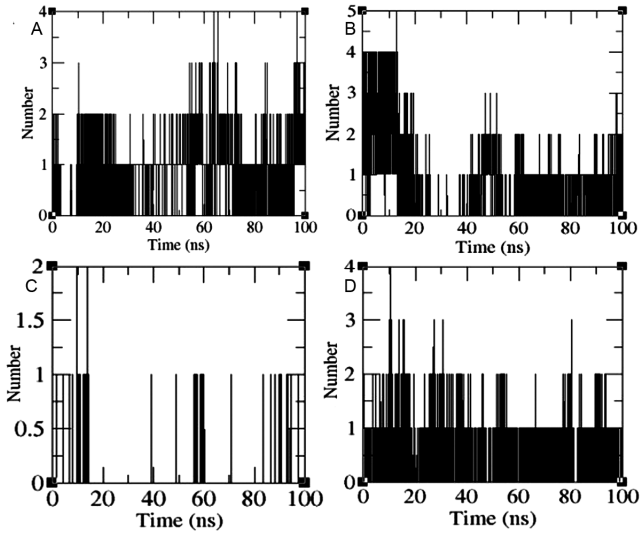

Fig. S3 — Hydrogen bond analysis of proteins -Hit 3 complex. (A)- MabA, (B)- FabD, (C)- KasA; and (D)- HadAB

Table S1 — Preliminary phytochemical analysis for crude petroleum ether extract of *Vitex negundo*

S. No	Phytochemical test	Petroleum ether extract
1	Alkaloid	++
2	Saponins	-
3	Steroids	-
4	Terpenoids	++
5	Tannins	-
6	Flavonoids	-
7	Anthraquinones	-
8	Fats and fixed oils	++
9	Coumarins	-
10	Anthocyanins	-
11	Betacyanin	-

* ++ indicates presence and – indicates absence.