Supplementary material:

Table 1: XP Docking of available drug molecules with PknG of *M. tuberculosis*

S. No	Compounds	Glide Score	Glide Energy	H Bond Interaction	Bond Distance(DH…A) Å
1	Ciproflaxin	-4.40	-31.959	(NH…O)A:GLU 233	2.853
2	Kanamycin	-6.91	-48.195	(OH…O)A:SER 239	3.252
				(NH…O)A:VAL 235	3.125
3	Isoniazid	-6.63	-28.956	(NH…O)A:ILE 292	2.459
				(NH…O)A:VAL 235	2.965
4	Ethionamide	-5.31	-26.184	(NH…O)A:GLU 233	2.698
5	Prothionamide	-5.82	-29.590	(NH…O)A:GLU 233	3.124
6	Pyrazinamide	-4.54	-27.236	(NH…O)A:GLU 233	2.568
				(NH…O)A:VAL 235	2.867
7	Amino salicylic acid	-5.19	-24.377	(NH…O)A:GLU 233	3.214
				(NH…O)A:VAL 235	3.312
8	Cycloserine	-4.34	-21.498	(NH…O)A:VAL 235	2.134
9	Streptomycin	-4.94	-44.669	A:LYS 241 (NH…O)	2.142
10	Ethambutol	-4.40	-31.959	(OH…O)A:GLY 237	3.217
				(NH…O)A:VAL 235	3.152

Table 2: XP Docking of bioactive compounds from *W somnifera* with PknG of *M. tuberculosis*

S. No	Compounds	Glide Score	Glide Energy	H Bond Interaction	Bond Distance (DH…A) Å
	AX20017	-5.63	-40.423	A:VAL 235 (NH…O)	3.381
				(NH…0) A:GLU 233	3.327
1	**Withanolide D**	**-7.63**	**-42.901**	**A:GLN 238 (NH…O)**	**2.779**
				A:VAL 235 (NH…O)	**3.068**
				A:SER 239 (OH…O)	**3.109**
2	Withanolide A	-4.51	-40.724	A:GLN 238 (NH…O)	3.005
3	**Withanolide E**	**-7.86**	**-48.905**	**A:VAL 235 (NH…O)**	**3.094**
				(OH…O) A:GLY 237	**2.739**
4	**Withanolide F**	**-7.69**	**-47.077**	**A:SER 293 (NH…O)**	**3.375**
				A:VAL 235 (NH…O)	**2.739**
5	4β-Hydroxywithanolide E	-6.46	-48.767	A:HIS 159 (NH…O)	2.980
				(OH…O) A:GLY 237	2.828
6	Withaferin A	-6.84	-36.108	(OH…O) A:ILE 292	2.849
				A:VAL 235 (NH…O)	2.935
7	Diacetate 2-phenylcarbonate withaferin A	-4.75	-41.948	-	-
8	2,3 dihydro withaferin A	-4.58	-34.799	A:SER 239 (OH…O)	2.856
				(OH…O) A:HIS 159	2.769
				A:LYS 241 (NH…O)	2.985
9	2,7 deoxy 2,3 dihydro withaferin A	-4.58	-34.799	A:SER 239 (OH…O)	2.856
				(OH…H) A:HIS 159	2.769
				A:LYS 241 (NH…O)	2.985
10	Deoxytetrahydroacetate withaferin A	-5.73	-41.078	A:GLN 238 (NH…O)	2.923
				(OH…O) A:GLY 237	2.979

Table 3: ADME results for the Withanolide compounds

S. No	Compounds	Molecular Weight (130.0 to 725.0)	Donor HB (0.0 to 6.0)	Accept HB (2.0 to 20.0)	QP LOG O/W (-2 to 6.5)	% Human Oral Absorption (>80% is high & <25% is poor)	Rule of Five
	Ligand	268.37	2.000	4.500	0.946	77.723	0
1	Withanolide D	454.61	1.000	8.700	3.481	100.00	0
2	Withanolide A	470.61	2.000	9.450	3.067	91.634	0
3	Withanolide E	486.60	3.000	9.250	3.153	95.431	0
4	Withanolide F	488.62	4.000	8.950	2.784	81.153	0
5	Withaferin	500.67	0.000	9.000	3.936	88.150	1