BIOINFORMATION

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Supplementary material:

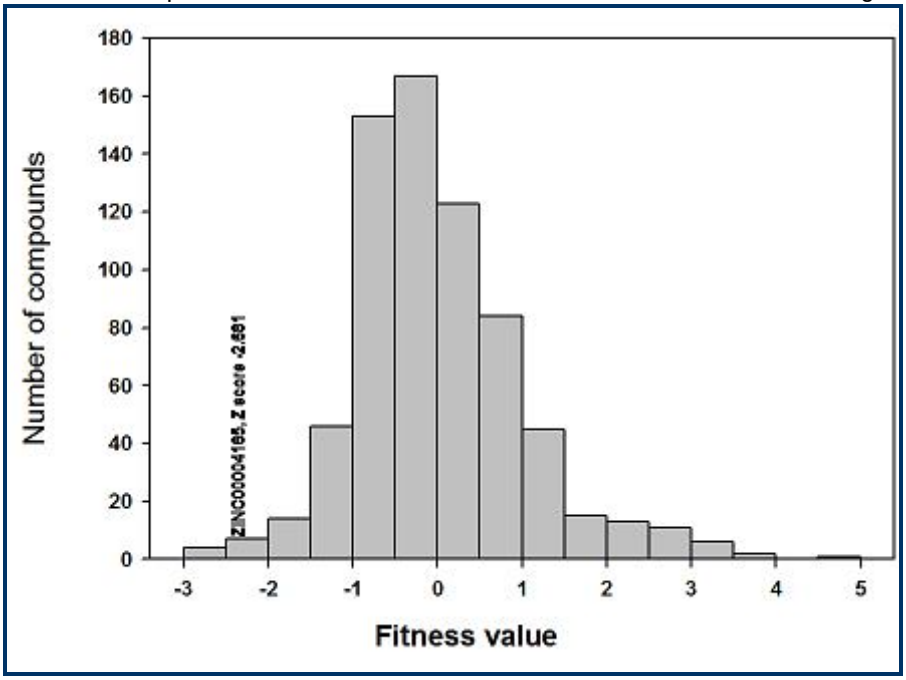
Table 1: Comparison of docking energy between ZINC00004165 and first line anti tuberculosis compounds.

	Autodock4.0	**Gemdockv2.0**
Compound	DE (kcal / mol)	Fitness value
ZINC00004165	-9.80	-113.255
ZINC04440911	-9.06	-109.309
Streptomycin	-8.19	-82.228
rifampicin	-8.00	-89.819
Ethambutol	-5.84	-54.669
Isoniazid	-4.53	-47.178
Pyrazinamide	-4.18	-49.158

Table 2: Comparison of Drug likeness properties of the selected ZINC compound ZINC00004165 and first line anti tuberculosis drugs

Molecular Properties							
Parameter	ZINC00004165	ZINC04440911	Streptomycin	Rifampicin	Ethambutol	Isoniazid	Pyrazinamide
miLogP	0.137	-2.417	-5.35	2.096	0.35	-0.969	-0.711
TPSA	67.535	99.104	336.45	216.662	64.51	68.013	68.878
natoms	25	37	40	59	14	10	9
MW	333.371	523.566	581.58	822.953	204.314	137.142	123.115
nON	6	9	19	16	4	4	4
nOHNH	0	1	16	6	4	3	2
nviolations	0	1	3	3	0	0	0
nrotb	5	6	9	5	9	1	1
volume	297.461	435.502	497.249	756.019	221.064	122.562	106.003
Drug Likness							
Parameter	ZINC00004165	ZINC04440911	Streptomycin	rifampicin	Ethambutol	Isoniazid	Pyrazinamide
GPCR ligand	-1.44	-0.17	-0.67	-3.59	0.21	-1.37	-1.51
Ion channel modulator	-0.66	-0.4	-1.15	-4.65	0.07	-1.53	-1.64
Kinase inhibitor	-1.56	-0.16	-0.76	-4.33	-0.27	-0.67	-2.14
Nuclear receptor ligand	-1.89	-0.85	-1.11	-4.55	-0.9	-2.56	-3.29

Graph 1: The distribution of Z score analysis of the compounds for finding of best compound with unique results. The compound ZINC00004165 produced Z score of -2.681 and located at one side tail of the histogram.



Graph 2: It represents the normal distribution analysis of the Z scores with respect to their probabilities of distribution of the compounds fitness values. The P value distributes on the Y axis and the Z score is on X axis. The compound ZINC00004165 shows Z score of -2.681 with P value of 0.003.