Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Formulation and Evaluation of *β*-Cyclodextrin-mediated Inclusion Complexes of Isoniazid Scaffolds: Molecular Docking and *In Vitro* Assessment of Antitubercular Properties

Lincy Tom, Christy Rosaline Nirmal, Azger Dusthackeer, B. Mahizhaveni and M.R.P. Kurup

Table S1. Changes in the chemical shifts of pure *β*-CD, HBIH/BDIH and *β*-CD inclusion complexes

Protons	*β*-CD	*β*-CD/HBIH	*β*-CD/BDIH	HBIH/BDIH
H-1	5.72	5.72	5.72	-
H-2	3.35	3.35	3.35	-
H-3	3.66	3.65	3.65	-
H-4	3.33	3.33	3.33	-
H-5	3.59	3.57	3.57	-
H-6	3.63	3.63	3.63	-
O–H (HBIH)	-	11.86	-	11.88
N–H (HBIH)	-	3.33	-	3.35
N–H (BDIH)	-	-	3.33	3.34

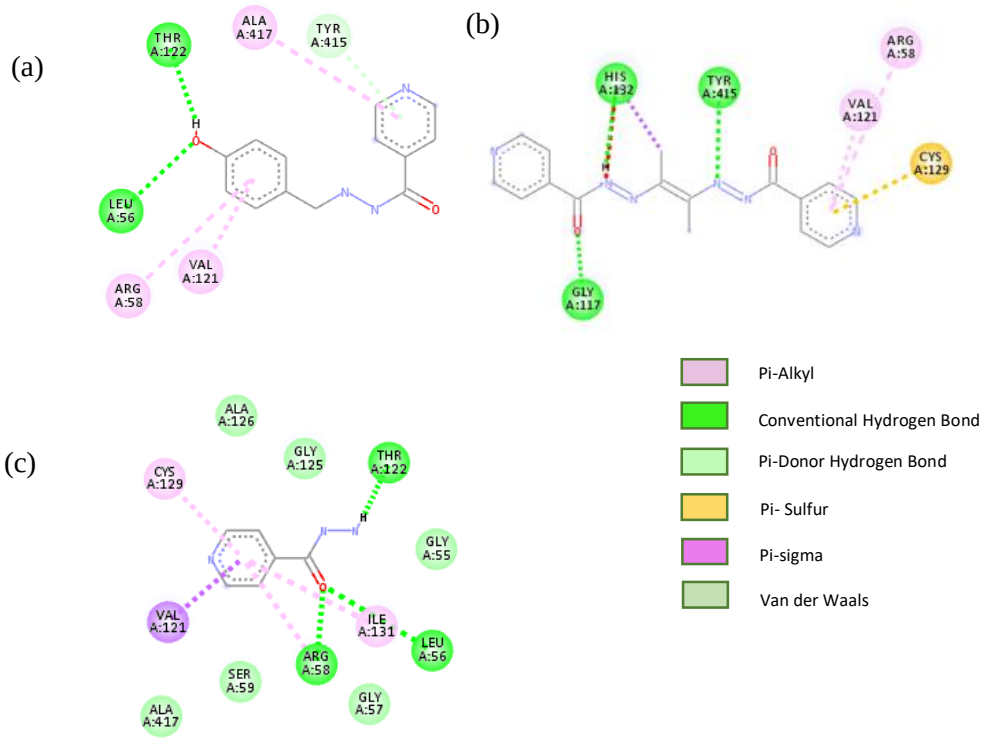

Fig S1. 2D interaction diagram of HBIH (a), BDIH (b) and IH (c) with DprE1.

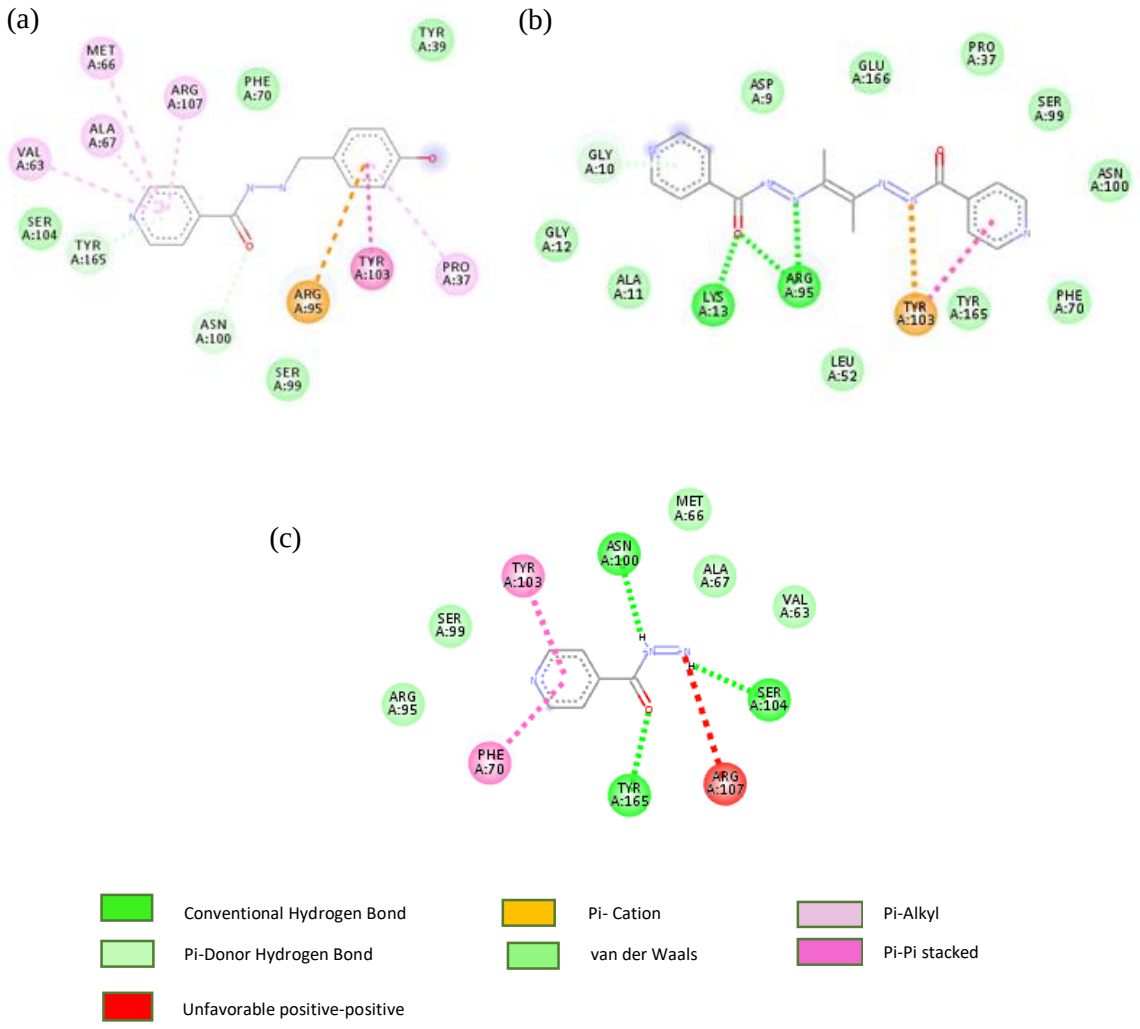

Fig S2. 2D interaction diagram of HBIH (a), BDIH (b) and IH (c) with TMPKinase.

Table S2. Preliminary anti-TB screening results for HBIH and BDIH

	Concentration (μg/mL)	Percentage of Inhibition
HBIH	100	85
	500	81
BDIH	100	94
	500	76

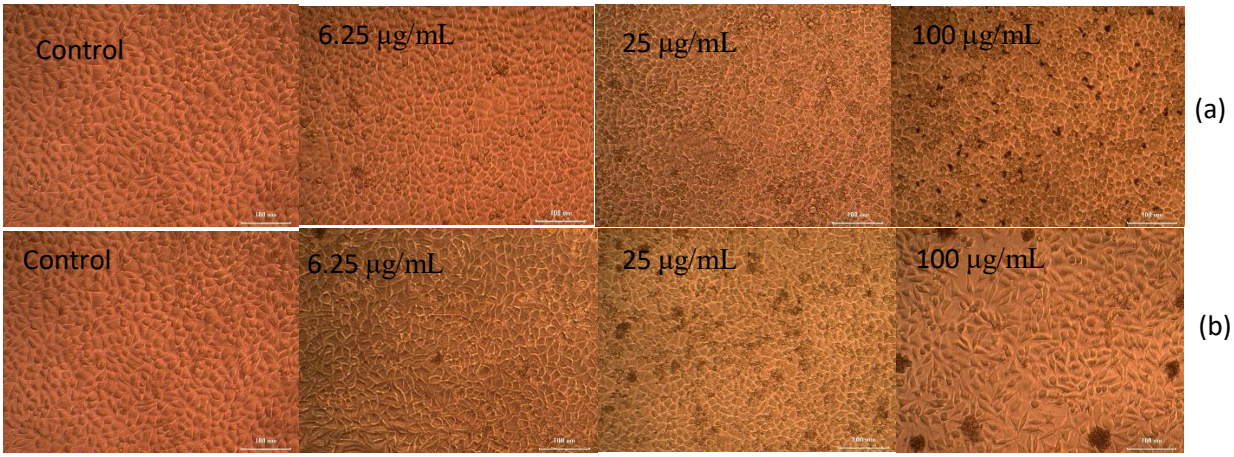

Fig. S3. Phase-contrast microscopy images of L929 fibroblast cell lines after incubation for 24 h with (a) *β*-CD/HBIH and (b) *β*-CD/BDIH at different concentrations 6.25,25,100 µg/mL.Positive control cells were treated with DMSO. The dark spots indicates apoptotic cells (scale: 100 µm).

Table S3. Molecular docking analysis of HBIH, BDIH and IH

Target	**DprE1**			**Thymidine Monophosphate Kinase**		
Target PDB id	**4FDN**			**1W2G**		
Ligand	HBIH	BDIH	IH	HBIH	BDIH	IH
Binding Energy (kcal/mol)	-7.34	-7.99	-5.18	-6.63	-7.41	-5.10
Inhibitory Constant	4.20 µM	1.38 µM	16.65 µM	13.76 µM	3.73 µM	18.86 µM
Internal Energy (kcal/mol)	-8.53	-9.48	0.02	-7.83	-8.90	-0.24
Torsional Energy (kcal/mol)	1.19	1.49	0.60	1.19	1.49	0.60
Electrostatic Energy (kcal/mol)	-0.14	-0.15	-0.13	-0.11	-0.52	-0.16
Unbound Extended Energy (kcal/mol)	-0.20	-0.61	0.02	-0.20	-0.60	-0.24
Hydrogen bonding Interactions	2	3	3	0	3	3
Interacting Residues	THR 122, LEU 56	HIS 132, TYR 415, GLY 117	ARG 58, LEU 56, THR 122	-	LYS 13, ARG 95	ASN 100, SER 104, TYR 165,
VanderWaal's Hydrogen bond Desolvation Energy (kcal/mol)	-8.39	-9.33	-5.65	-7.71	-8.38	-5.54