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An insight into the antimycobacterial and antioxidant potentials of INH-Schiff base complexes and *insilico* targeting of MtKasB receptor of *M.tuberculosis*

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SUPPLEMENTARY INFORMATION

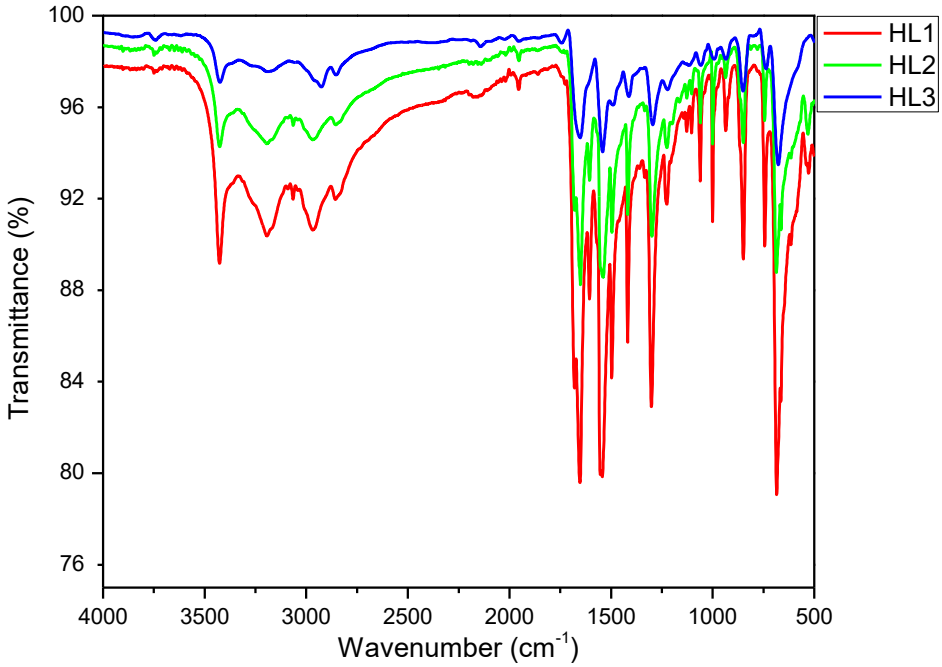

Figure S1: FT-IR spectra of INH-Schiff base ligands (1-3)

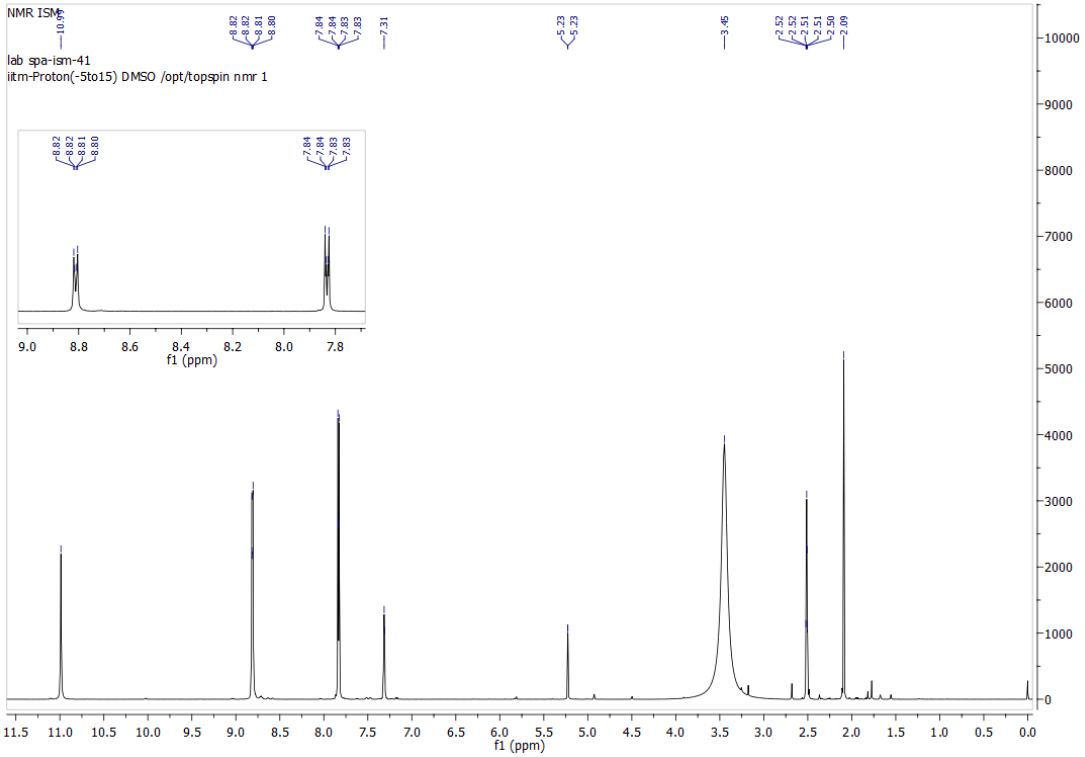

Figure S2: ^{1}H NMR spectrum of INH-Schiff base ligand (1)

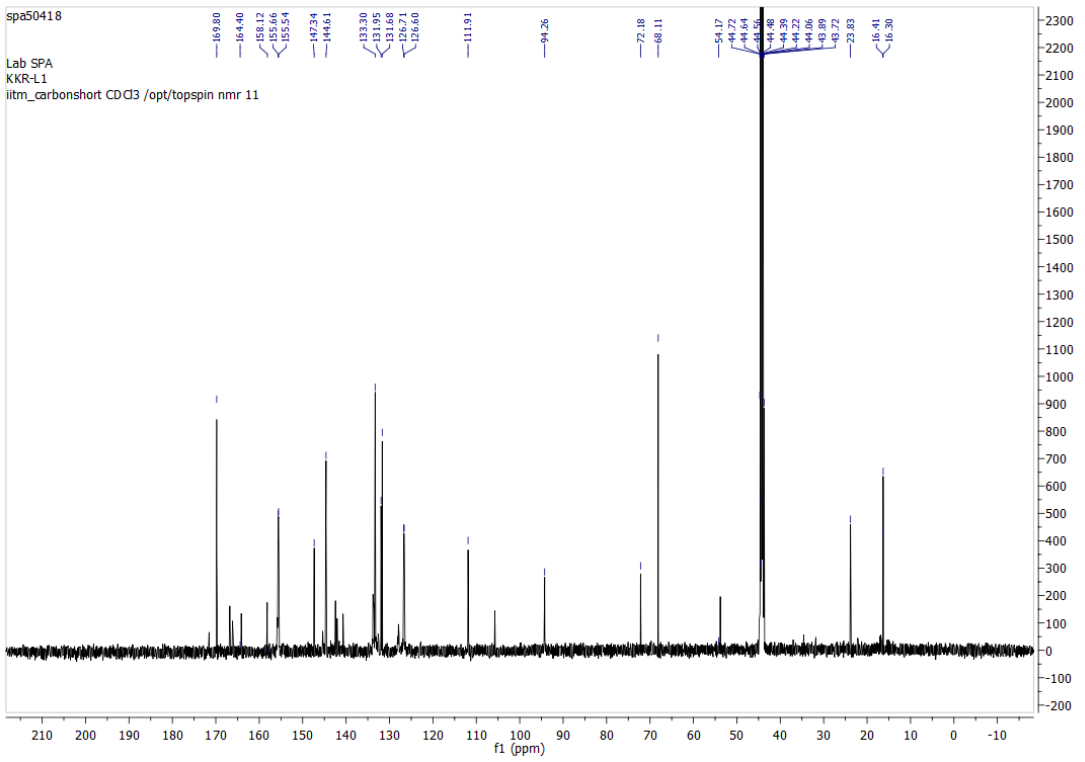

Figure S3: ^{13}C NMR spectrum of INH-Schiff base ligand (1)

^{1}H NMR signals			
Schiff base ligands	N-**H** (amide proton)	-C**H$_2$**- (methylene proton)	-C=N-C**H$_3$** (methyl proton)
HL^{1}	10.99	3.45	2.09
HL^{2}	11.00	3.50	2.09
HL^{3}	9.96	3.29	2.04

^{13}C NMR signals				
Schiff base ligands	**C=O** (amide)	**C=N** (azomethine)	**C=O** (ester)	**-CH$_3$** (methyl)
HL^{1}	164.40	155.66	169.80	16.30
HL^{2}	162.68	155.35	174.04	22.49
HL^{3}	165.03	155.60	166.79	18.02

Table S1: NMR data of INH-Schiff base ligands

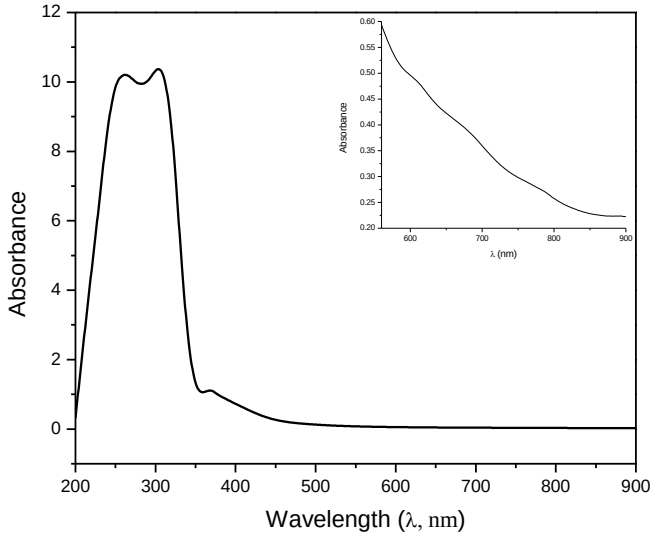

Figure S4: Electronic spectrum of Ni(II) complex (4)

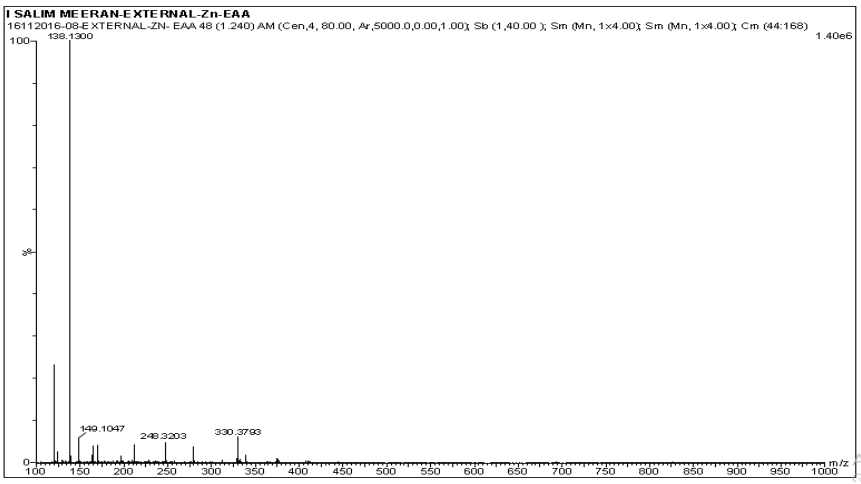

Figure S5: Mass spectrum of Zn(II) complex (12)

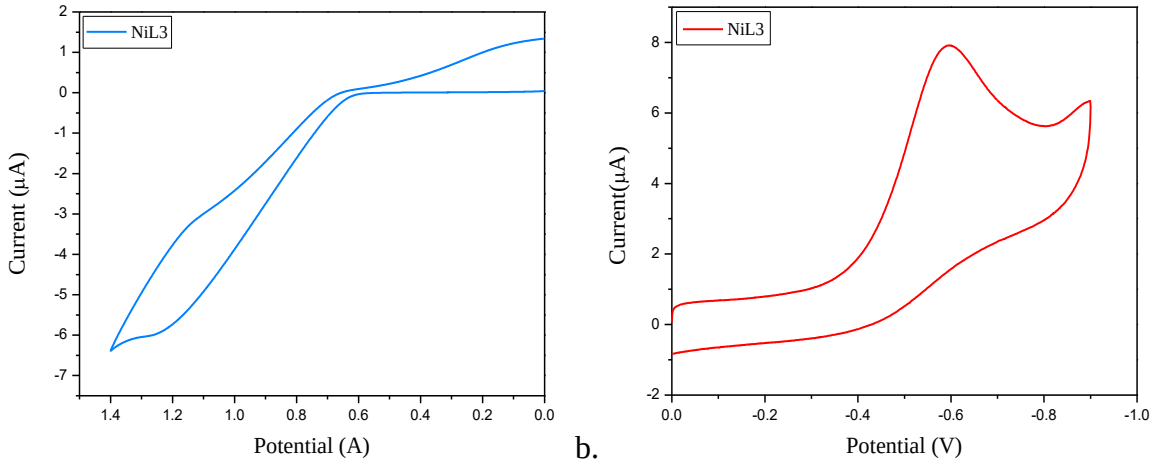

Figure S6: Cyclic voltammograms of Ni(II) complex (6): (a) anodic region and (b) cathodic region

INH-SB	LUMO / HOMO	Energy (AU)	ΔE (eV)	INH-SB	LUMO / HOMO	Energy (AU)	ΔE (eV)
HL1	83	0.03856	5.13	**NiL1**	173	-0.27515	1.67
	82	-0.14986			172	-0.33645	
HL2	63	0.03944	5.13	**NiL2**	133	-0.30884	1.05
	62	-0.14909			132	-0.34756	
HL3	67	0.0399	5.11	**NiL3**	141	-0.29692	1.14
	66	-0.14785			140	-0.33872	
CoL1	173	-0.26134	2.66	**ZnL1**	93	-0.28754	2.48
	172	-0.35901			92	-0.37863	
CoL2	132	-0.29079	1.98	**ZnL2**	73	-0.32782	1.87
	131	-0.36362			72	-0.3967	
CoL3	141	-0.24354	2.52	**ZnL3**	77	-0.29159	2.42
	140	-0.33615			76	-0.3804	

Table S2: Energies of HOMO and LUMO of INH-SB ligands and complexes

Compound	Scavenging Activity (%)				
	10 µg	20 µg	40 µg	80 µg	100 µg
1	54.3	82.3	99.1	99.8	99.9
2	70.7	88.8	99.5	99.7	99.9
3	77.2	91.3	99.4	99.8	99.9
6	92.0	97.8	97.8	99.6	99.8
7	95.7	98.4	98.3	98.2	98.5
8	96.9	97.5	97.7	98.8	99.1
11	74.4	93.7	99.8	99.9	99.8
12	51.2	85.9	98.6	99.7	99.7
13	55.6	96.1	100.0	100.0	100.0
16	95.3	99.2	99.2	99.4	99.7
17	94.5	99.6	99.7	99.8	99.6
18	89.2	99.7	99.8	99.8	99.8
Ascorbic Acid	99.0	99.4	100.0	100.0	100.0

Table S3: ABTS Radical Scavenging Activity of INH-Schiff base ligands (1-5) and complexes (6-20) at 10 – 100 µg/mL concentrations

Compound	Scavenging Activity (%)				
	0.5 µg	**1 µg**	**2 µg**	**4 µg**	**8 µg**
1	5.4	7.2	9.6	10.8	15.3
2	7.7	6.2	8.6	14.7	24.1
3	1.9	1.9	2.5	3.7	5.9
4	9.8	18.0	34.7	61.4	88.5
5	16.9	24.0	42.1	78.2	94.3
6	13.8	27.6	52.5	82.7	89.8
7	0.8	3.5	5.4	9.9	16.8
8	3.9	4.9	6.5	10.0	17.2
9	2.4	4.8	7.9	12.5	27.0
10	-14.5	-6.6	10.9	27.9	69.0
11	23.4	30.9	44.5	70.8	95.2
12	17.5	25.1	51.6	84.3	99.8
Ascorbic Acid	6.8	7.0	7.3	8.3	10.7

Table S4: ABTS Radical Scavenging Activity of INH-Schiff base ligands (1-5) and complexes (6-20) at 0.5 – 8 µg/mL concentrations

Sample code	Sample	RLU		Log_{10} RLU	
		5 µg	10 µg	5 µg	10 µg
1	HL^1	64	64	1.81	1.81
2	HL^2	60	68	1.78	1.83
3	HL^3	140684	120401	5.15	5.08
6	NiL^1	71232	43598	4.85	4.64
7	NiL^2	103539	43234	5.02	4.64
8	NiL^3	75777	546	4.88	2.74
11	CoL^1	74984	73603	4.87	4.87
12	CoL^2	68790	87652	4.84	4.94
13	CoL^3	77244	79237	4.89	4.90
16	ZnL^1	53072	1385	4.72	3.14
17	ZnL^2	57476	22645	4.76	4.35
18	ZnL^3	18366	3545	4.26	3.55
Control 1		121025		5.08	
Control 2		132684		5.12	

Table S5: Anti-mycobacterial activity in RLU and log_{10} RLU of INH-Schiff base ligands (1-3) and their complexes (4-12) using LRP assay