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

Supporting Information

Enolato-bridged dinuclear Cu(II) complex with a coumarin-assisted precursor : Spectra, magnetism and biological study

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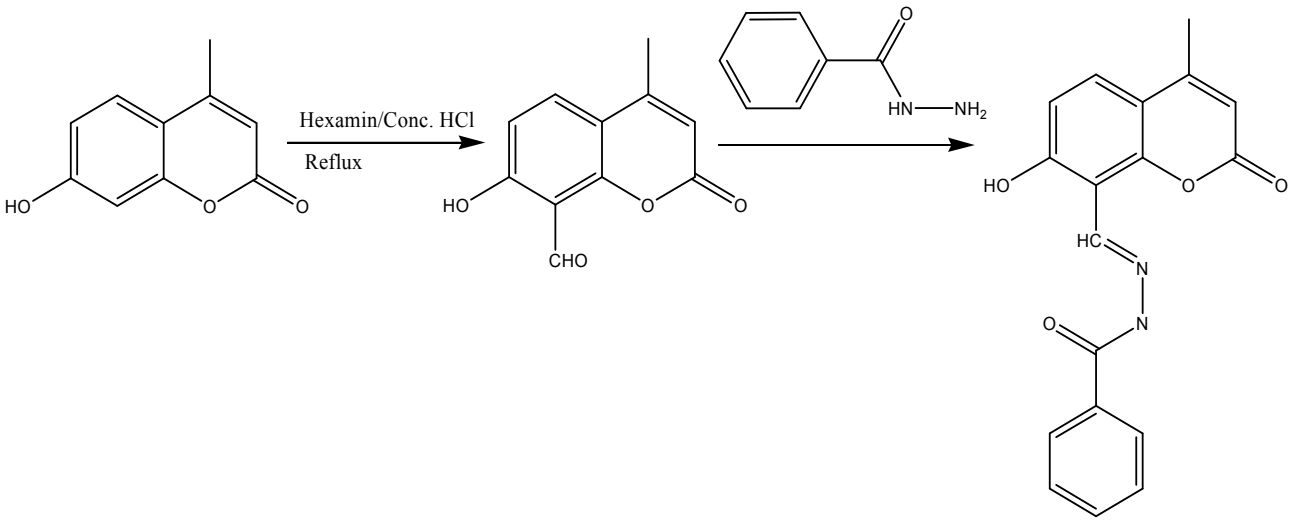

Scheme SI. Synthesis of the ligand, H_2L.

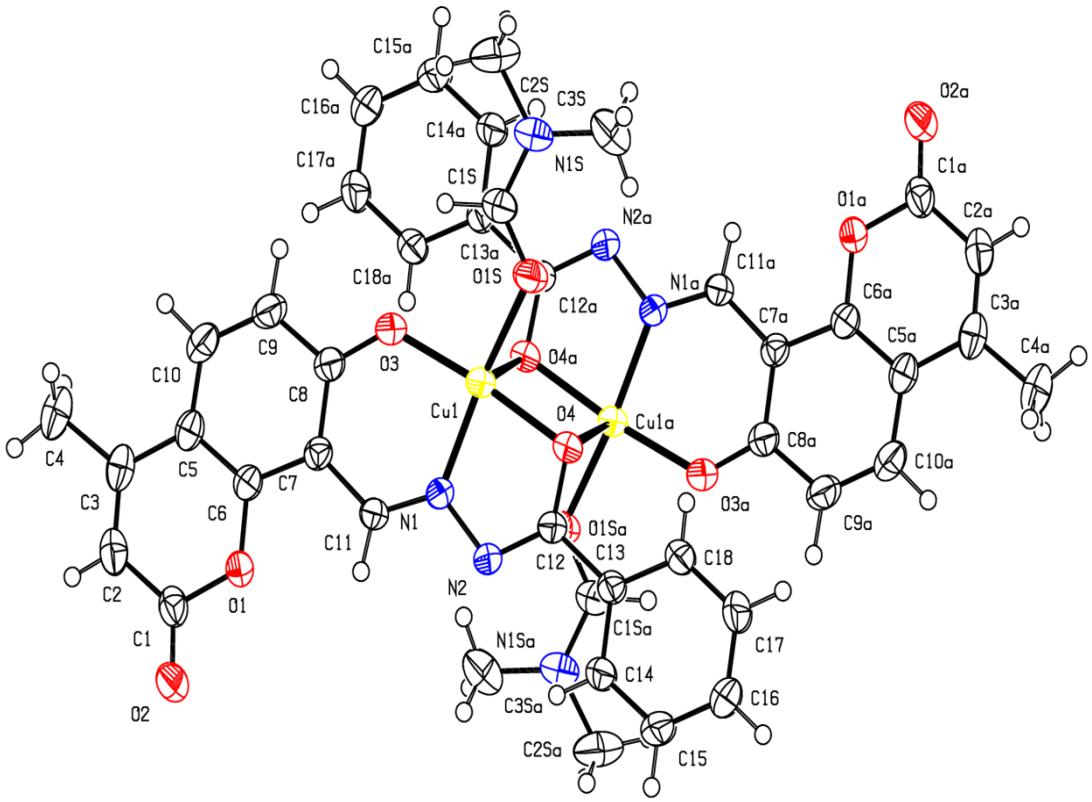

Figure S1. Ortep view of complex **1** with the atom labeling scheme. Ellipsoids are drawn at the 40% probability level.

UV-Vis Spectra

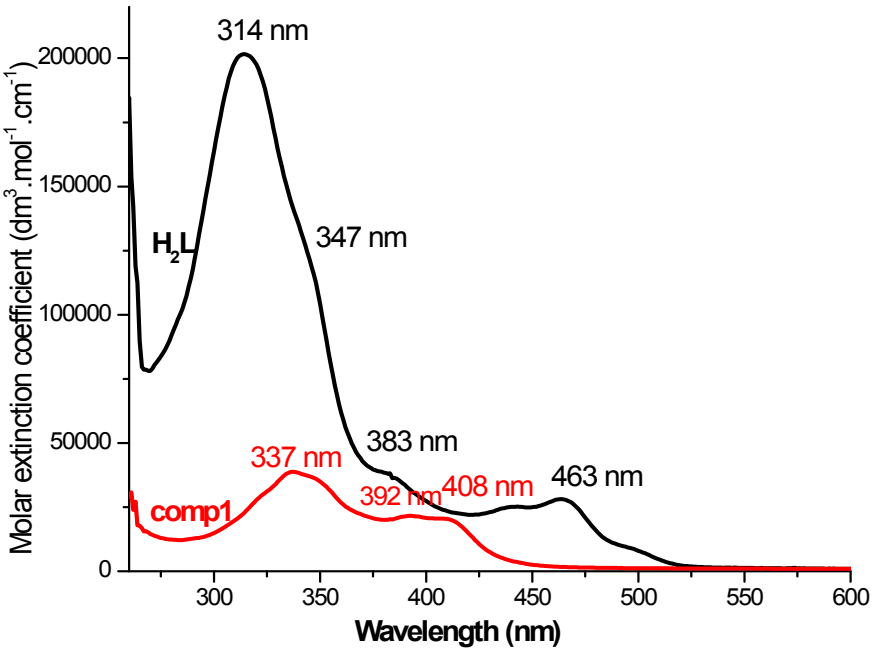

Figure S2. UV-Vis spectra of complex **1** and the ligand, H_2L.

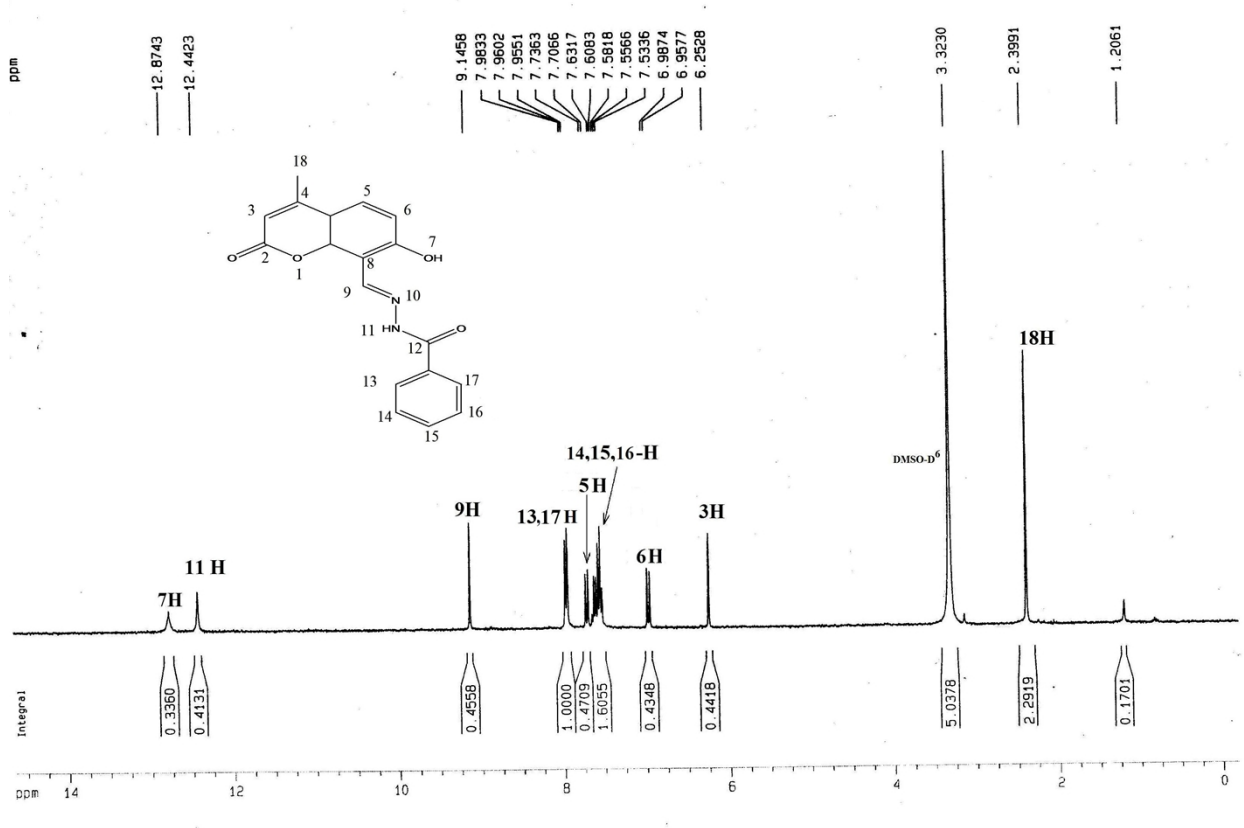

Figure S3. ^{1}H NMR Spectra of H_2L.

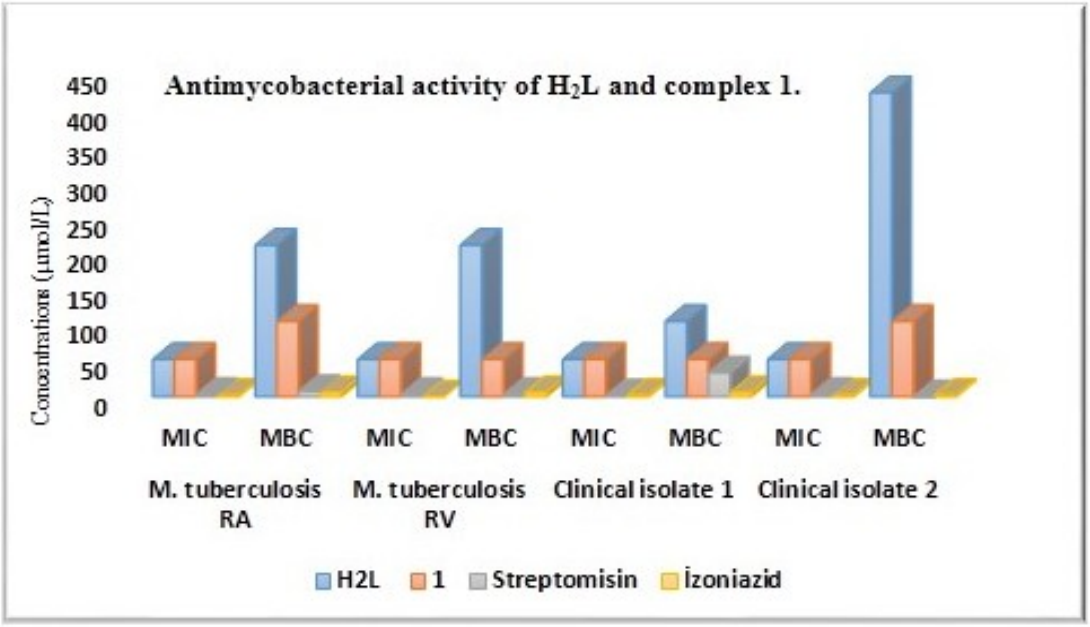

Figure S4. Antimycobacterial activity of H_2L, complex **1** and standard drugs.

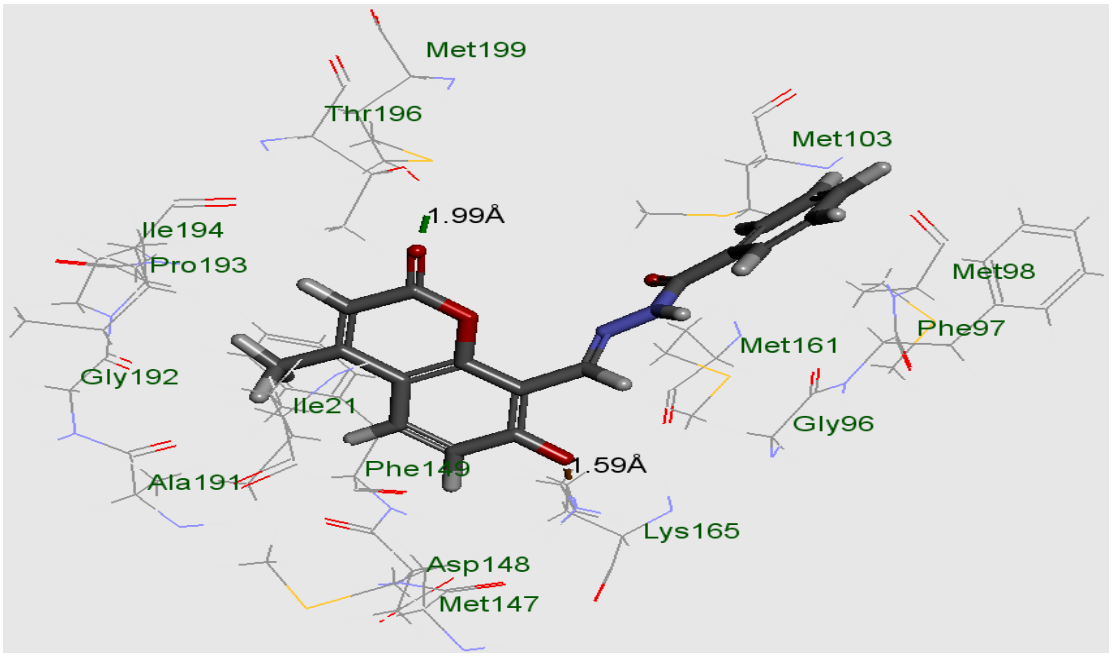

Figure S5. Best docked pose of ligand (H_2L) (2D view) and enoyl acyl carrier protein reductase (PDB id 4U0K) of *M. tuberculosis* $H37R_v$.

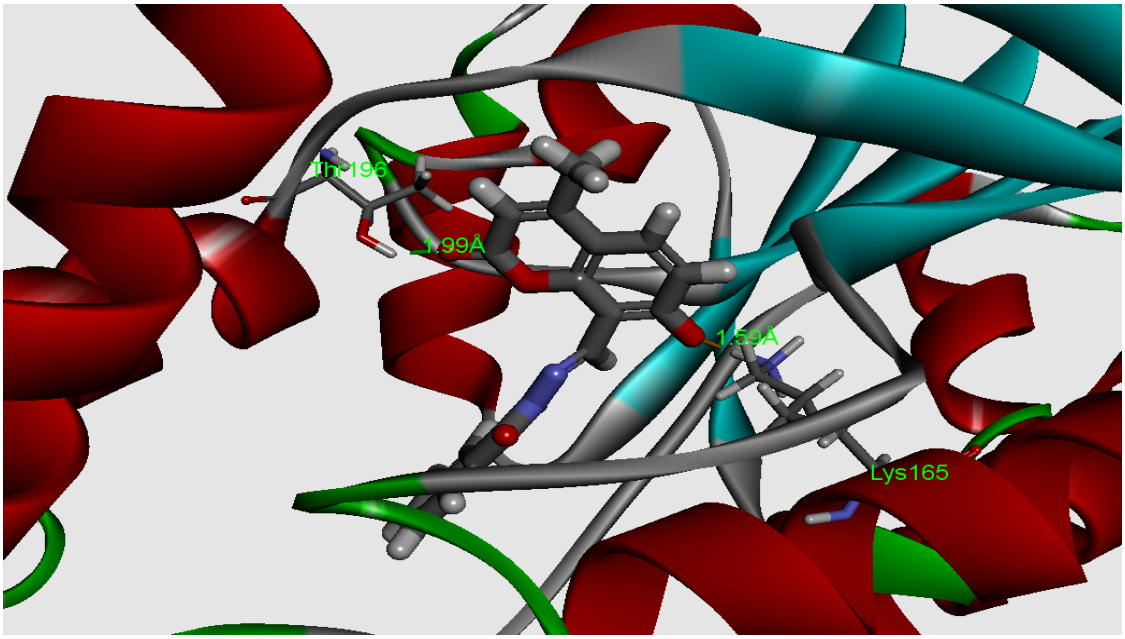

Figure S6. Best docked pose of ligand (H_2L) (3D view) and enoyl acyl carrier protein reductase (PDB id 4U0K) of *M. tuberculosis* $H37R_v$.

Table S1. Selected Orbital Energies and Orbital Composition for α and β spin state of $Cu_2[(L)_2(DMF)_2]$ (**1**).

	α-molecular orbitals of **1**				β-molecular orbitals of **1**			
MO-α	Energy (eV)	DMF	L	Cu	Energy (eV)	DMF	L	Cu
LUMO+5	-0.77	12	87	01	-1.67	00	99	01
LUMO+4	-0.84	09	91	00	-1.7	00	99	01
LUMO+3	-1.67	00	100	00	-1.96	00	99	01
LUMO+2	-1.7	00	99	01	-1.98	01	96	03
LUMO+1	-1.99	00	99	01	-2.73	04	36	60
LUMO	-2.02	01	98	01	-2.75	04	34	62
HOMO	-5.51	00	98	02	-5.45	01	96	03
HOMO-1	-5.7	00	98	02	-5.66	00	98	02
HOMO-2	-6.03	00	99	01	-6.01	00	99	01
HOMO-3	-6.07	00	99	01	-6.04	00	99	01
HOMO-4	-6.37	04	82	14	-6.72	01	87	12
HOMO-5	-6.4	05	80	15	-6.89	01	97	02

Table S2. Selected electronic excitation for $Cu_2[(L)_2(DMF)_2]$ (**1**).

Excitation energy (eV)	Wavelength (nm)	f	Key Transitions	Character
α molecular orbitals				
3.0553	405.80	0.5762	(40%) HOMO→LUMO	ILCT
3.2725	378.87	0.1586	(45%) HOMO-1→LUMO+1	ILCT
3.4080	363.81	0.0350	(39%) HOMO→LUMO+2	ILCT
3.6000	344.40	0.9203	(16%) HOMO-2→LUMO+1	ILCT
3.6977	335.30	0.3549	(45%) HOMO-1→LUMO+3	ILCT
3.7110	334.10	0.0395	(33%) HOMO-2→LUMO+1	ILCT
3.9342	315.14	0.0314	(23%) HOMO-5→LUMO	ILCT
4.1335	299.95	0.1194	(26%) HOMO-4→LUMO+3	ILCT

Table S3. Selected electronic excitation for $Cu_2[(L)_2(DMF)_2]$ (**1**).

Excitation energy (eV)	Wavelength (nm)	f	Key Transitions	Character
β-molecular orbitals				
2.3616	524.99	0.0046	(31%) HOMO→LUMO+1	ILCT, LMCT
2.8512	434.85	0.0025	(58%) HOMO-3→LUMO+1	ILCT, LMCT
3.0553	405.80	0.5762	(46%) HOMO→LUMO+2	ILCT
3.2725	378.87	0.1586	(31%)HOMO-1→LUMO+3	ILCT
3.3723	367.66	0.0959	(42%) HOMO→LUMO+4	ILCT
3.4395	360.47	0.0201	(27%) HOMO-9→LUMO+1	ILCT, LMCT
4.1335	299.95	0.1194	(26%) HOMO-4→LUMO+3	ILCT

Table S4. Antimycobacterial activity (MIC and MBC, μg/ml) of H_2L and complex **1**.

Compounds	**The minimal inhibitory concentration (MIC)**				**The minimal bactericidal concentration (MBC)**			
	M. tuberculosis RA		*M. tuberculosis* RV		Clinical isolate 1		Clinical isolate 2	
	MIC	MBC	MIC	MBC	MIC	MBC	MIC	MBC
H_2L	52.96	211.84	52.96	211.84	52.96	105.92	52.96	423.68
1	52.96	105.92	52.96	52.96	52.96	52.96	52.96	105.92
Concentrations of antimycobacterial drugs (μmol/L)								
Streptomisin	4.30	8.53	4.30	4.30	2.59	34.29	4.30	-
İzoniazid	3.37	6.81	0.86	6.81	3.37	6.81	3.37	3.37

Table S5. Details of the docking studies of H_2L with the enoyl acyl carrier protein reductase of *M. tuberculosis* H37Rv (PDB ID: 4U0K).

Compound	CDOCKER interaction energy	Binding energy (Kcal/mol)	Ligand energy (Kcal/mol)	Protein energy (Kcal/mol)	Energy of protein ligand complex (Kcal/mol)
4U0K@ H_3L	-40.12	-209.91	0.72	-10272.18	-10481.40

$Energy_{Binding} = Energy_{Complex} - Energy_{Ligand} - Energy_{Receptor}$

Table S6. Details of the interactions present in the most stable protein-ligand complex for the ligand, H_2L.

Compound	Hydrogen bonds				Ionic interaction			
	No. of hydrogen bonds	End 1	End 2	Bond Distances Å	No. of ionic interactions	End 1	End 2	Bond Distances Å
H_2L	1	Thr196	O-atom of carbonyl group in coumarin moiety	1.99	1	Lys165	O-atom of -OH group in coumarin moiety	1.59