Supplementary Information

Self-assembly of Sm(III) Schiff base complexes: Crystal structure, luminescence and antibacterial inhibition activity

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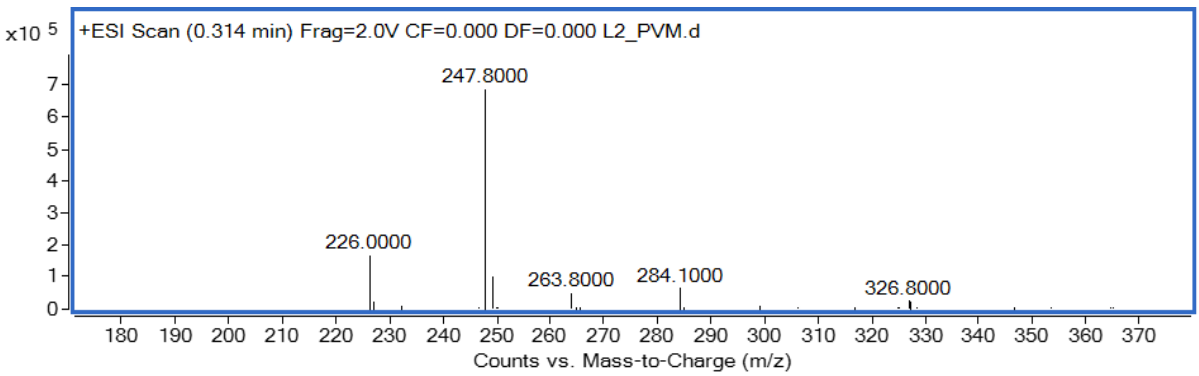
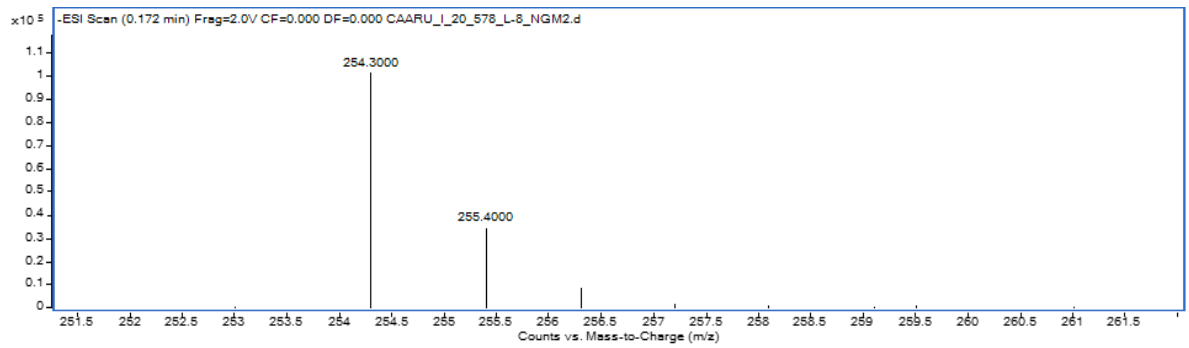
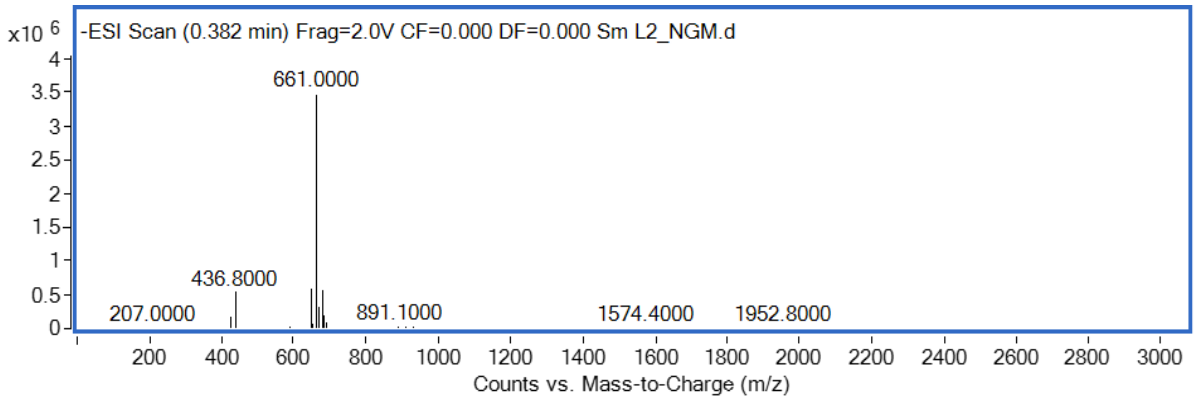
Ligand 1 *m/z* [225+1]{**1**}$^{+}$.



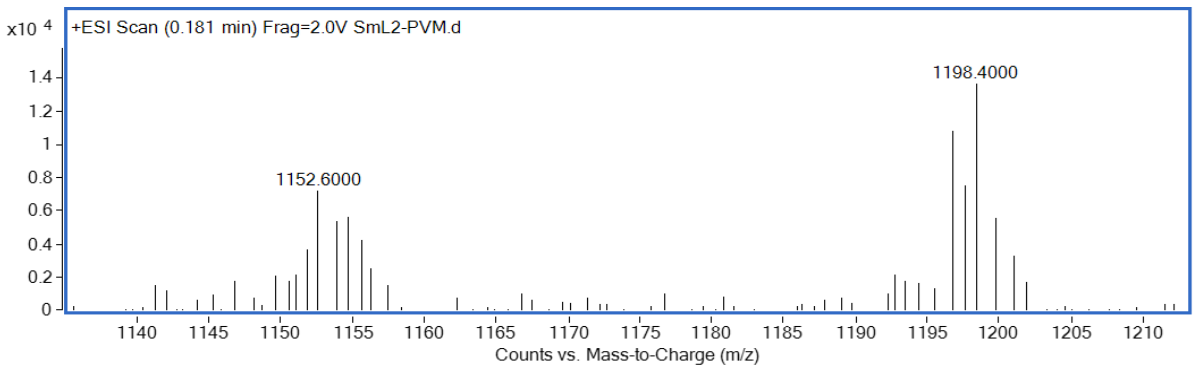
Ligand 2 *m/z* 255{**2**}$^{+}$.



Sm1 *m/z* 891{[Sm(**1**)(hfac)$_2$(Cl)(MeOH)]}$^-$ and 661 {[Sm(**1**)$_2$(MeOH)$_2$}$^-$.



Sm2 *m/z* 1152.40 {[Sm(**2**)$_2$(Tba)$_2$(NO$_3$)]}$^+$.



Gd2 *m/z* 793{[Gd(**1**)$_2$(hfac)]}$^-$.

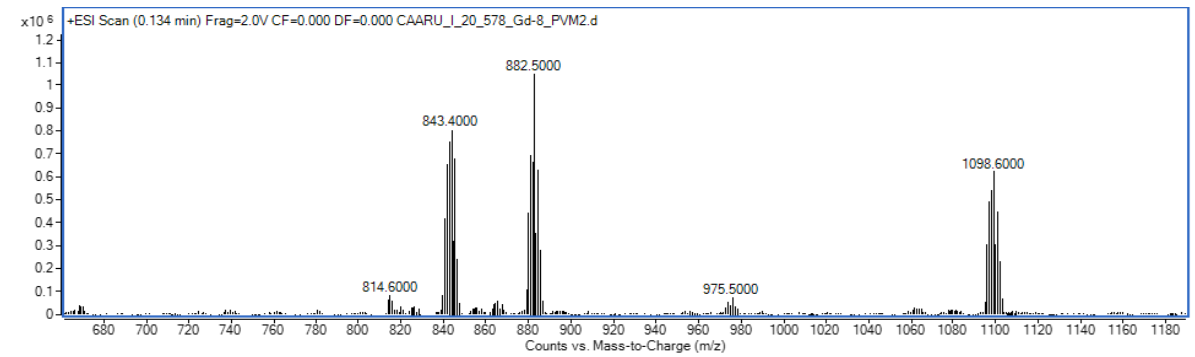
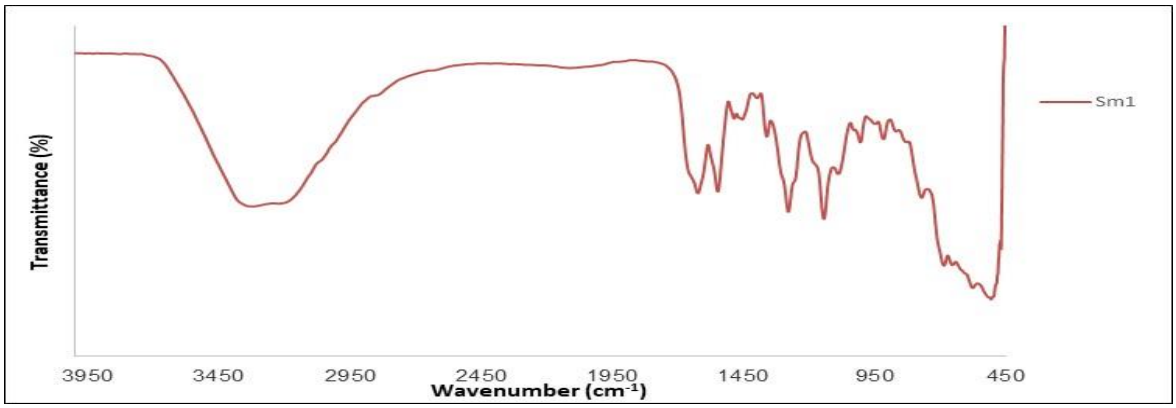


Figure S1. ESI-MS of Ligand **1**, Ligand **2**, **Sm1**, **Sm2** and **Gd1.**

(a)

(b)



(c)

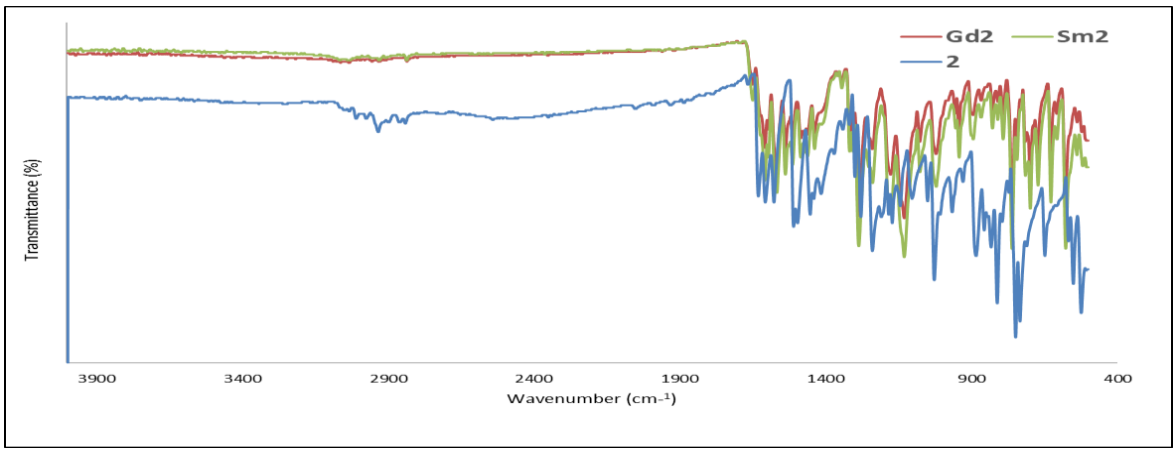
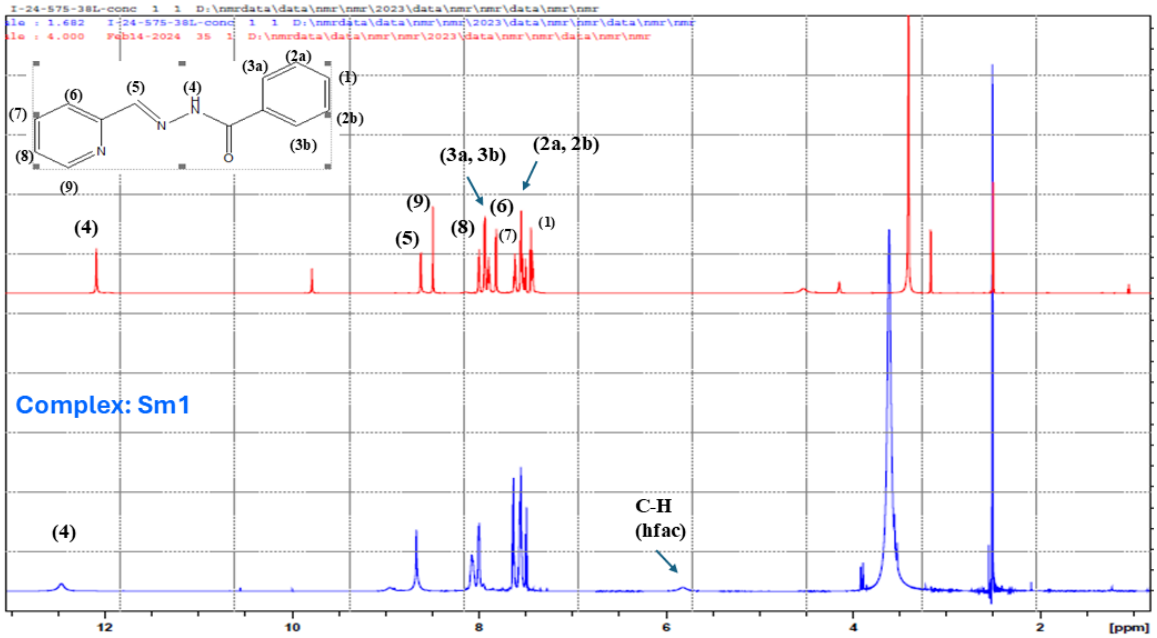


Figure S2: The solid-state FT-IR Spectra of (a) **1**, (b) **Sm1** and (c) **Sm2** & **Gd2**.

(a)



(b) .

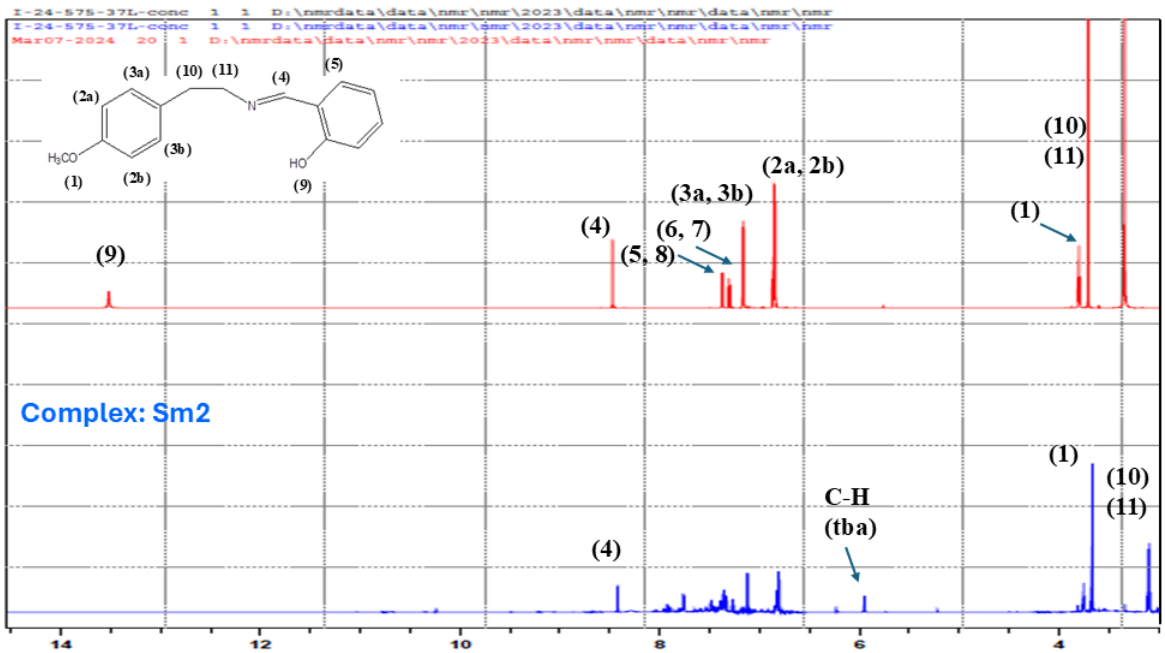


Figure S3: ^{1}H NMR (500 MHz) spectrum of (a) SB ligand **1** & **Sm1**, and (b) SB ligand **2** & **Sm2** in DMSO-d_6.

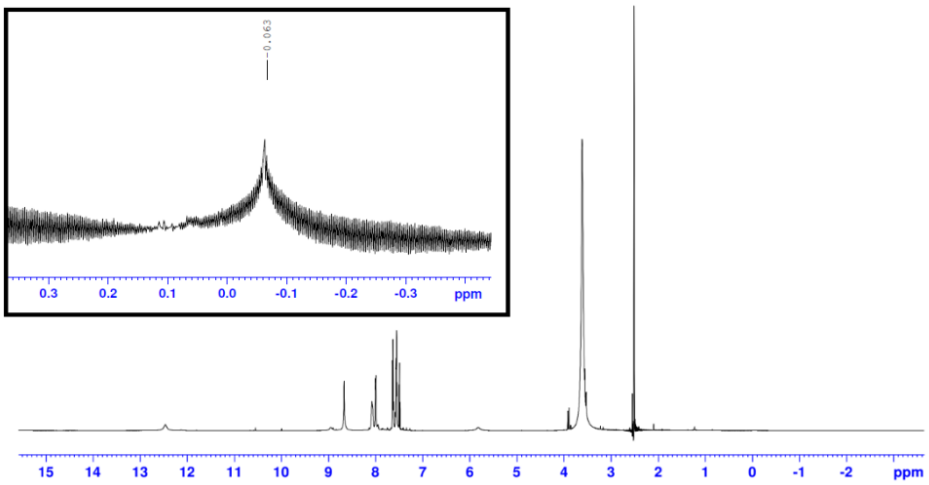


Figure S4: The paramagnetic ^{1}H NMR (500 MHz) spectrum of **Sm1** in DMSO-d_6. Inset: A weak signal appears at -0.063 ppm due to the paramagnetic nature of Sm(III).

In the next stage, it is necessary to investigate the feasibility of the mesocate assembly of **Sm1** in solution, using 2D COSY ^{1}H NMR in DMSO-d_6, Figure S5. Accordingly, the spectrum gives evidence to hydrogen interactions between the neighboring protons. The correlations of the peaks are unremarkable. The COSY spectrum revealed hydrogen interactions between the neighboring aromatic protons. No significant hydrogen interactions between the ligand's protons and the trapped water molecules inside the assembly were seen. We conclude that the **Sm2** molecules aggregate randomly in DMSO.

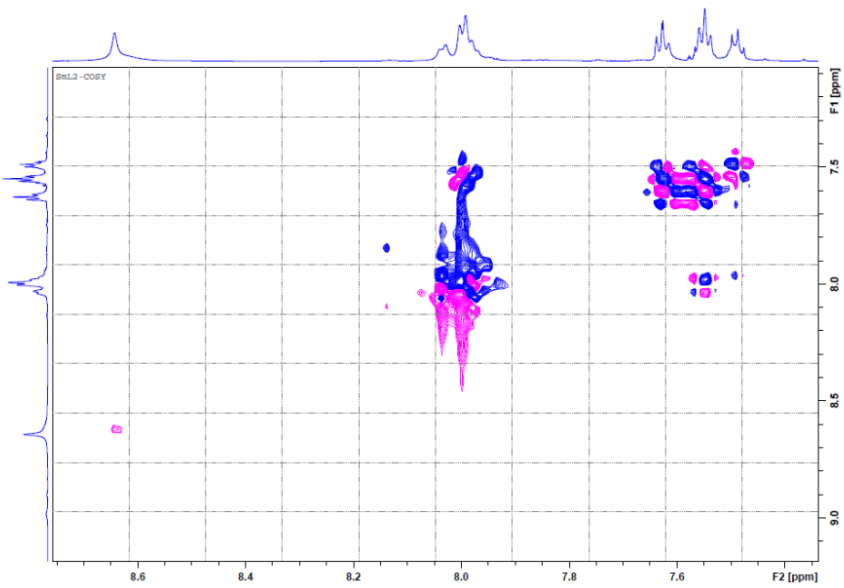


Figure S5: The COSY ^{1}H NMR (500 MHz) spectrum of **Sm1** in DMSO-d_6.

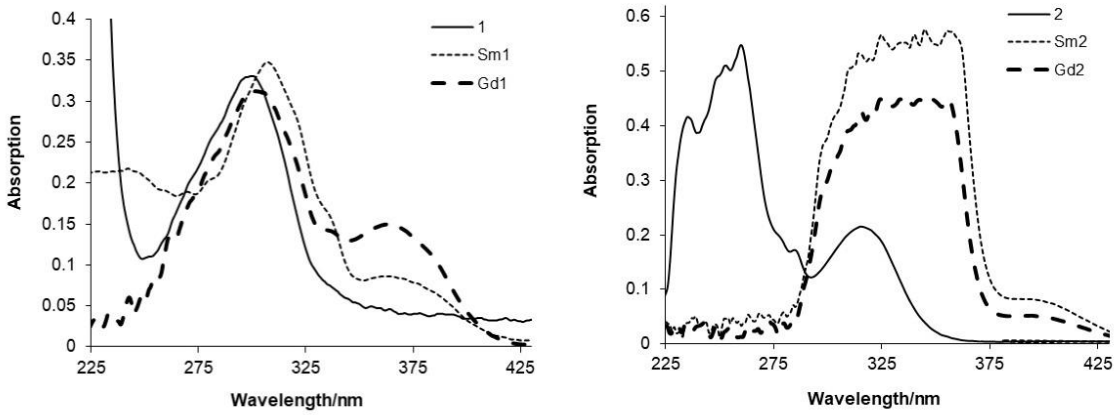


Figure S6: The UV/Vis absorption spectra of the SB ligands and their Sm(III) and Gd(III) complexes in DCM (1 x10^{-5} M) at 298 K.

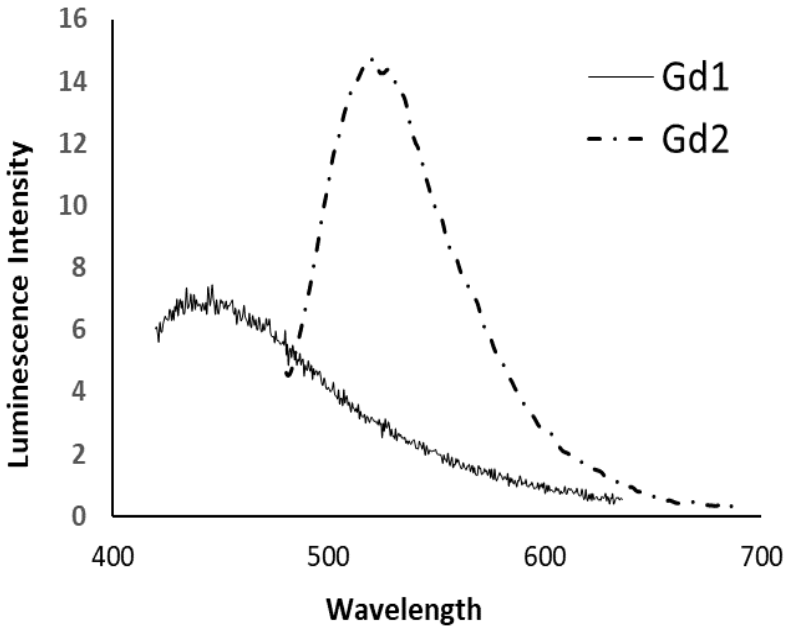


Figure S7: The phosphorescence spectra of **Gd1** and **Gd2** in ethanol (5 x10^{-5} M) at 77 K excited at 372 and 397 nm respectively.

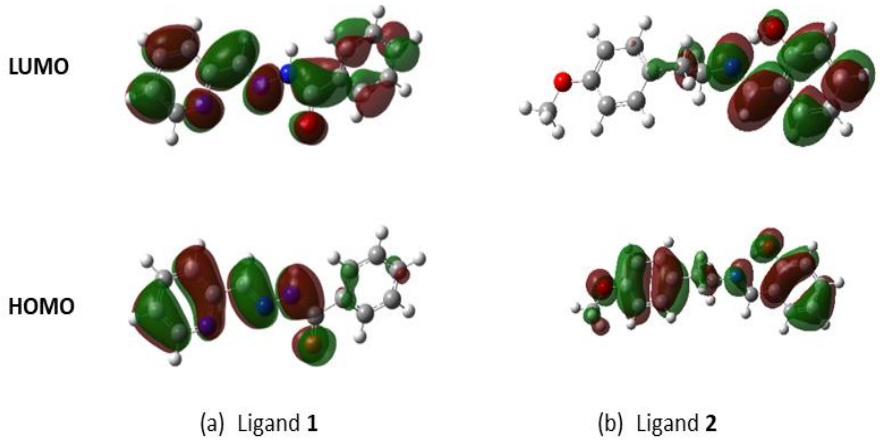


Figure S8: Plots of the relevant molecular orbitals from HOMO and LUMO orbitals of the singlet states of ligands (a) **1** and (b) **2** in the gas-phase.

Summary of TD DFT results: The ligands are optimized from ground state geometries at the UAPFD function 6-311+g(2d,p) basis in the gas-phase.

Ligand 1

Singlet Excitation energies									
HOMO is 59	59								
No.	Energy (cm-1)	(eV)	Wavelength (nm)	Osc. Strength	Symmetry	Major con	Minor con	Minor contribs	
1	20792.97318	2.577912815	480.9317029	0	3.000-A	HOMO(A)	HOMO(A)->L+2(A) (2%), HOMO(B)->L+2(B) (2%)		
2	27890.65215	3.457883054	358.5430683	0	3.000-A	H-1(A)->LI	H-4(A)->LI	H-4(A)->LUMO(A) (2%), H-1(A)->LUMO(A) (9%), H-4(B)->LUMO(B) (2%), H-1(B)->LUMO(B) (9%)	
3	28808.5111	3.571679206	347.11964	0	3.000-A	H-2(A)->LI	H-2(A)->L	H-7(A)->LUMO(A) (2%), H-6(A)->L+2(A) (3%), H-5(A)->LUMO(A) (2%), H-5(A)->L+3(A) (2%), H-4(	
4	31299.95773	3.880568759	319.4892494	0	3.000-A	H-1(A)->LI	H-7(A)->LI	H-7(A)->L+1(A) (2%), H-6(A)->L+1(A) (2%), H-5(A)->L+1(A) (3%), H-5(A)->L+2(A) (2%), H-4(A)->L	
5	32111.35148	3.981165357	311.416354	0	3.000-A	H-5(A)->L	H-7(A)->LI	H-2(A)->LUMO(A) (2%), H-2(B)->LUMO(B) (2%)	
6	32963.07296	4.086761785	303.3697742	0.0049	1.000-A	H-2(A)->LI	H-2(A)->L	H-2(A)->L+2(A) (2%), H-1(A)->L+7(A) (3%), H-2(B)->L+2(B) (2%), H-1(B)->L+7(B) (3%)	
7	33462.33015	4.148659692	298.8435042	0	3.000-A	HOMO(A)	H-7(A)->LI	H-4(A)->LUMO(A) (2%), H-4(A)->L+2(A) (4%), H-4(A)->L+3(A) (2%), H-3(A)->LUMO(A) (6%), H-2(	
8	33472.0088	4.149859651	298.7570916	0.81	1.000-A	HOMO(A)->LUMO(A		H-3(A)->LUMO(A) (6%), H-2(A)->LUMO(A) (8%), H-3(B)->LUMO(B) (6%), H-2(B)->LUMO(B) (8%)	
9	33855.92871	4.197458042	295.369242	0	3.000-A	H-6(A)->LI	H-6(A)->L	H-5(A)->L+2(A) (2%), H-4(A)->L+3(A) (3%), H-3(A)->LUMO(A) (7%), H-3(A)->L+3(A) (2%), H-2(A)-	
10	34097.89504	4.227457027	293.2732354	0.0895	1.000-A	H-2(A)->LI	H-4(A)->LI	H-3(A)->LUMO(A) (5%), H-3(B)->LUMO(B) (5%)	

E T	-741.983	Eh		Eh_eV	27.21141
E S	-742.102	Eh		nm_eV	1239.8
DE	0.118492	Eh			
T	3.224344	eV		384.5123	

Ligand 2

Excitation energies							
HOMO is 68	68						
No.	Energy (cr	(eV)	Waveleng	Osc. Strength	Symmetry	Major con	Minor contribs
1	23727.22	2.941701	421.4569	0	3.000-A	H-2(A)->LUMO(A) (11%), H-1(A)->LUMO(A) (13%), HOMO(A)->LUMO(A) (22%), H-2(B)->LUMO(B) (11%), H-1(B)->LUM	
2	28171.33	3.492682	354.9708	0	3.000-A	H-2(A)->LI	H-2(A)->L+2(A) (3%), H-1(A)->L+2(A) (4%), HOMO(A)->LUMO(A) (3%), HOMO(A)->L+2(A) (3%), H-2(B)->L+
3	28888.36	3.581579	346.1602	0	3.000-A	H-3(A)->L	H-1(A)->L+1(A) (2%), HOMO(A)->L+1(A) (3%), H-1(B)->L+1(B) (2%), HOMO(B)->L+1(B) (3%)
4	32292.02	4.003565	309.674	0	3.000-A	H-1(A)->L	H-1(A)->LUMO(A) (4%), H-1(A)->L+2(A) (2%), HOMO(A)->LUMO(A) (3%), HOMO(A)->L+3(A) (2%), H-1(B)->
5	32806.6	4.067362	304.8167	0	3.000-A	H-1(A)->L	H-2(A)->LUMO(A) (7%), H-1(A)->L+1(A) (2%), H-1(A)->L+3(A) (3%), HOMO(A)->L+1(A) (4%), H-2(B)->LUMO
6	32871.13	4.075362	304.2184	0.1744	1.000-A	H-1(A)->LUMO(A) (14%), HOMO(A)->LUMO(A) (33%), H-1(B)->LUMO(B) (14%), HOMO(B)->LUMO(B) (33%)	
7	33554.28	4.160059	298.0246	0	3.000-A	H-4(A)->LI	H-1(A)->LUMO(A) (2%), HOMO(A)->LUMO(A) (2%), H-1(B)->LUMO(B) (2%), HOMO(B)->LUMO(B) (2%)
8	34608.44	4.290755	288.9468	0.0313	1.000-A	H-1(A)->LUMO(A) (33%), HOMO(A)->LUMO(A) (15%), H-1(B)->LUMO(B) (33%), HOMO(B)->LUMO(B) (15%)	
9	34956.88	4.333953	286.0668	0	3.000-A	H-1(A)->LI	H-4(A)->LUMO(A) (6%), H-3(A)->L+1(A) (5%), H-2(A)->LUMO(A) (3%), H-4(B)->LUMO(B) (6%), H-3(B)->L+1(
10	36862.76	4.570245	271.2765	0	3.000-A	H-3(A)->L	H-1(A)->L+3(A) (7%), H-1(B)->L+3(B) (7%)

E T	-824.59	Eh		Eh_eV	27.21141
E S	-824.692	Eh		nm_eV	1239.8
DE	0.102237	Eh			
T	2.782019	eV		445.6475	

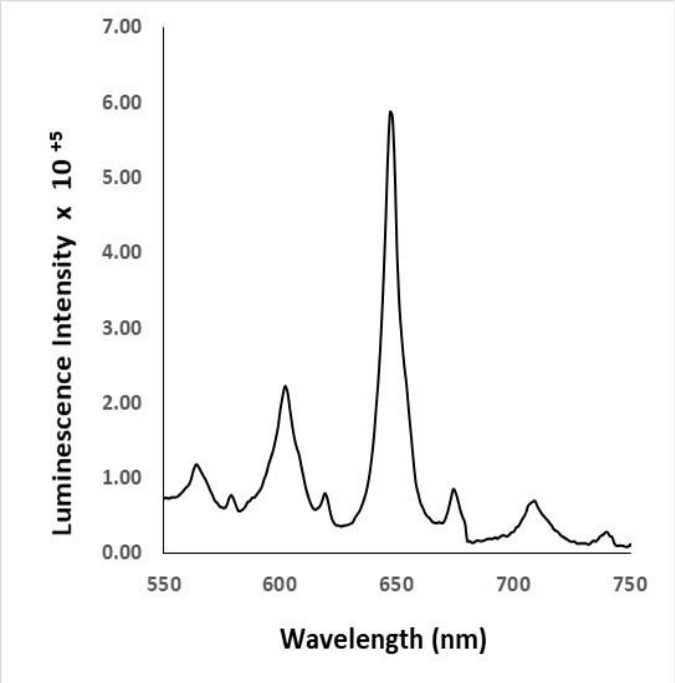


Figure S9: Room temperature luminescence spectra of **Sm2** (excited at 397 nm) in the solid state.

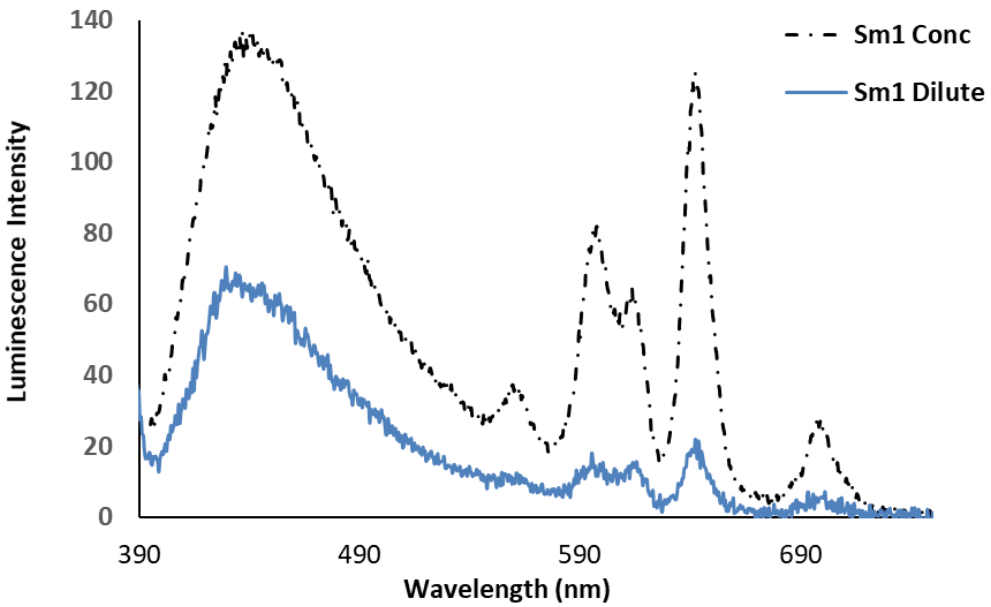


Figure S10: Room temperature luminescence spectra of **Sm1** (dotted) and **diluted-Sm1** (blue) (excited at 372 nm) in DMSO.

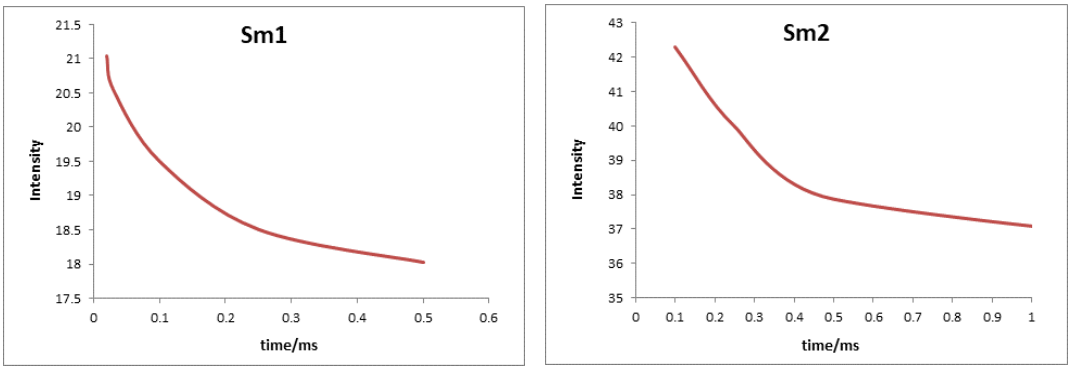


Figure S11: Room temperature luminescence *f-f* lifetime decays for **Sm1** (excited at 372 nm) and **Sm2** (excited at 397 nm) complexes in DMSO. IRF = 2.0.

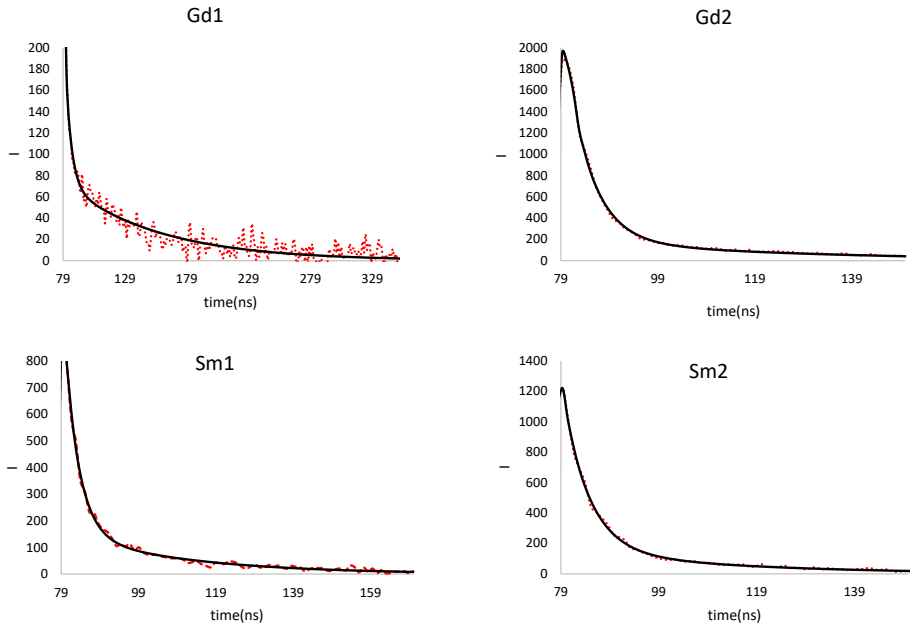


Figure S12: Room temperature emission lifetime decays at π-π* ligand based bands for the **Ln1** (excited at 372 nm) and **Ln2** (excited at 397 nm) complexes in DMSO. IRF = 2.0.

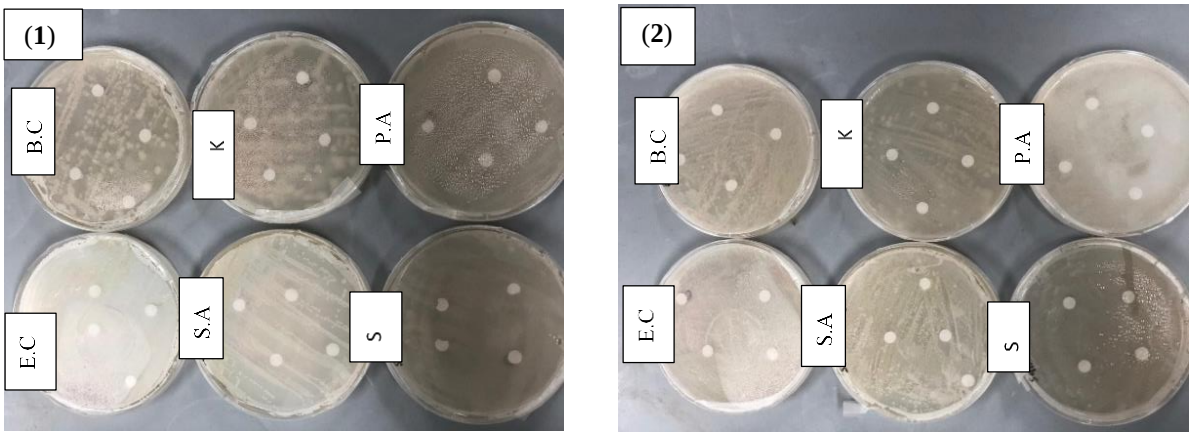


Figure S13: The Antibacterial tests of ligand **1** (left) and **2** (right) on B.C, K., P.A., E. coli, S.A. and S.