Supplementary Material for

A water-soluble Schiff base ligand and its Al(III) complex: optical properties, computational studies and photocatalytic performance

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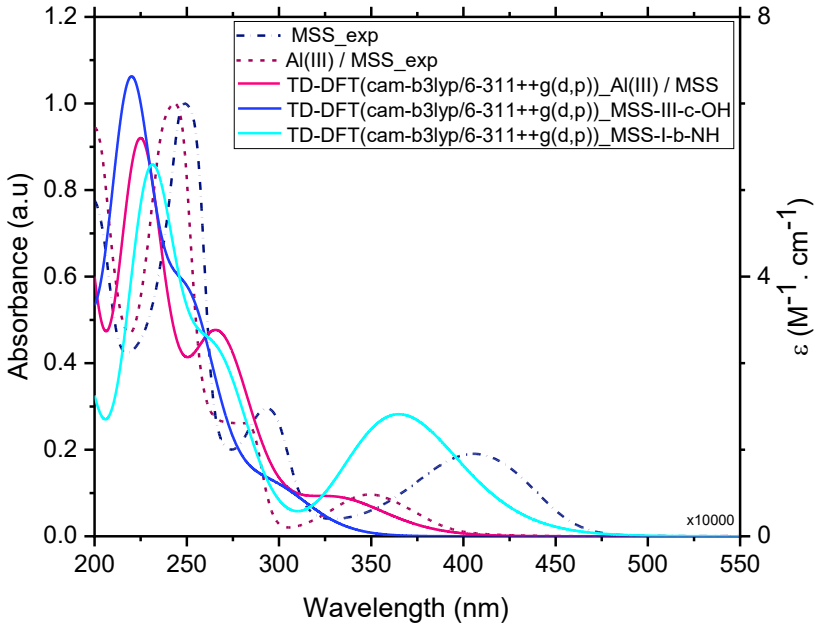

Figure S1. Experimental and calculated (TD-DFT CAM-B3LYP/6-311++G(d,p)) absorption spectra of **MSS** and **Al(III)/MSS** complex (H_2O).

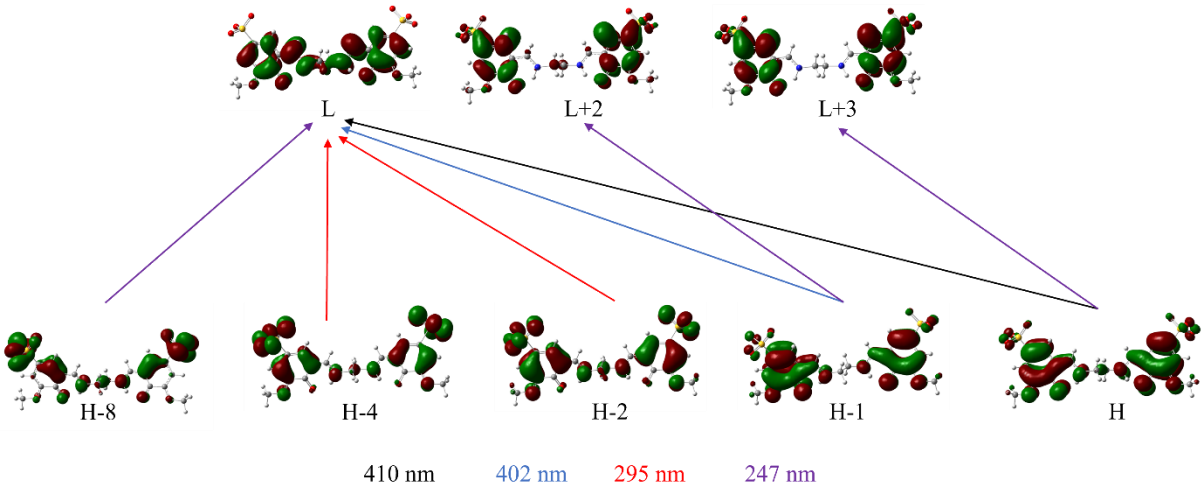

Figure S2. Diagram of the molecular orbitals involved in the main contributions to the UV-vis absorption spectrum of the I-b-NH conformer of **MSS** (TD-DFT B3LYP/6-311++G(d,p), IEFPCM (H_2O)).

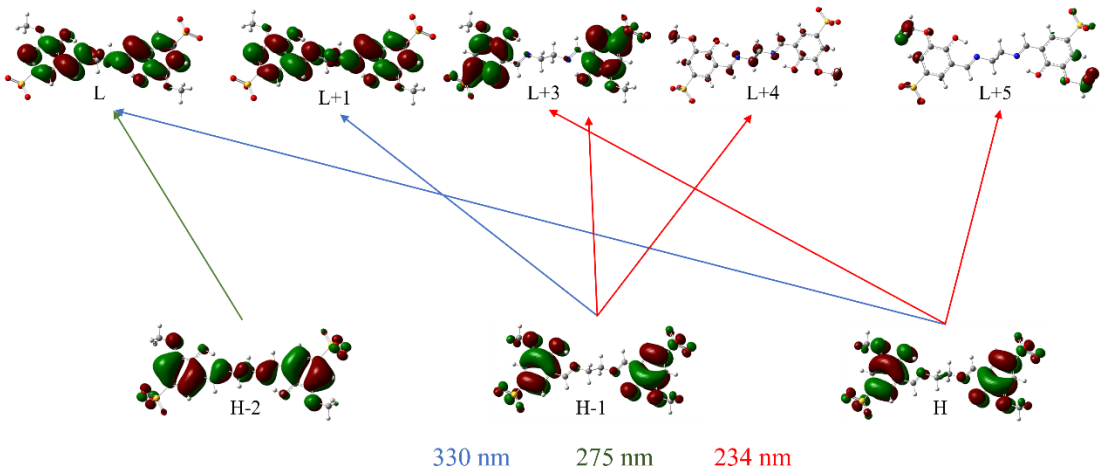

Figure S3. Diagram of the molecular orbitals involved in the main contributions to the UV-vis absorption spectrum of the **III-c-OH** conformer of **MSS** (TD-DFT B3LYP/6-311++G(d,p), IEFPCM (H_2O)).

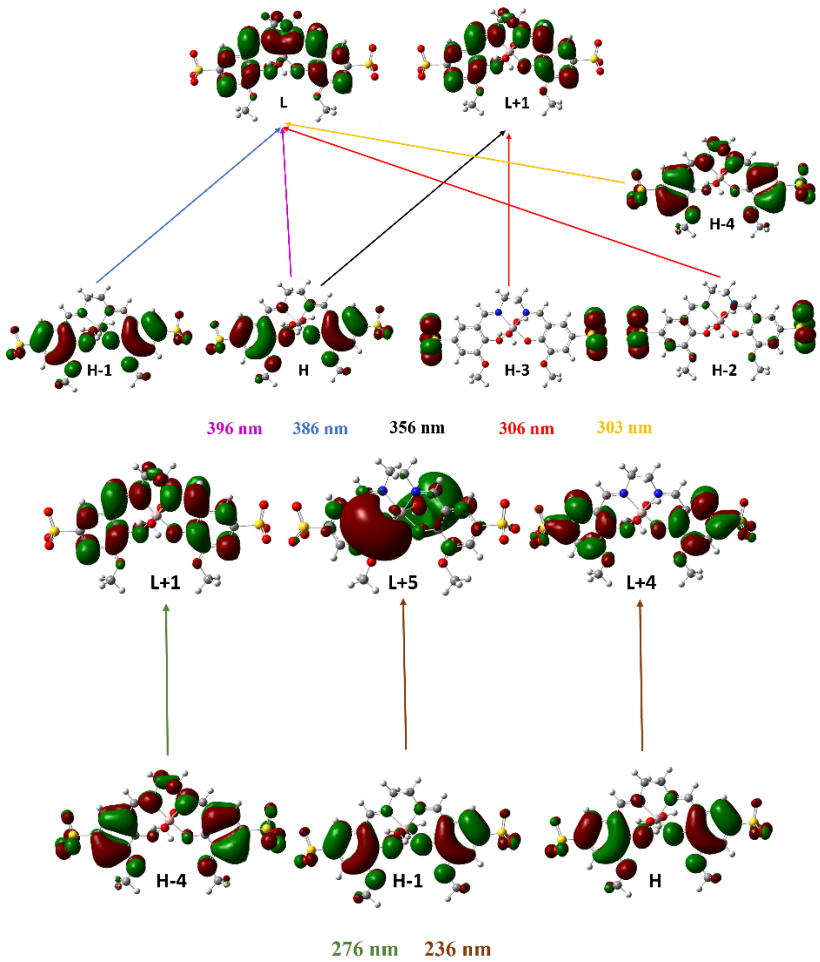

Figure S4. Diagram of the molecular orbitals involved in the main contributions to the UV-vis absorption spectrum of the **Al(III)/MSS** complex (TD-DFT B3LYP/6-311++G(d,p), IEFPCM (H_2O)).

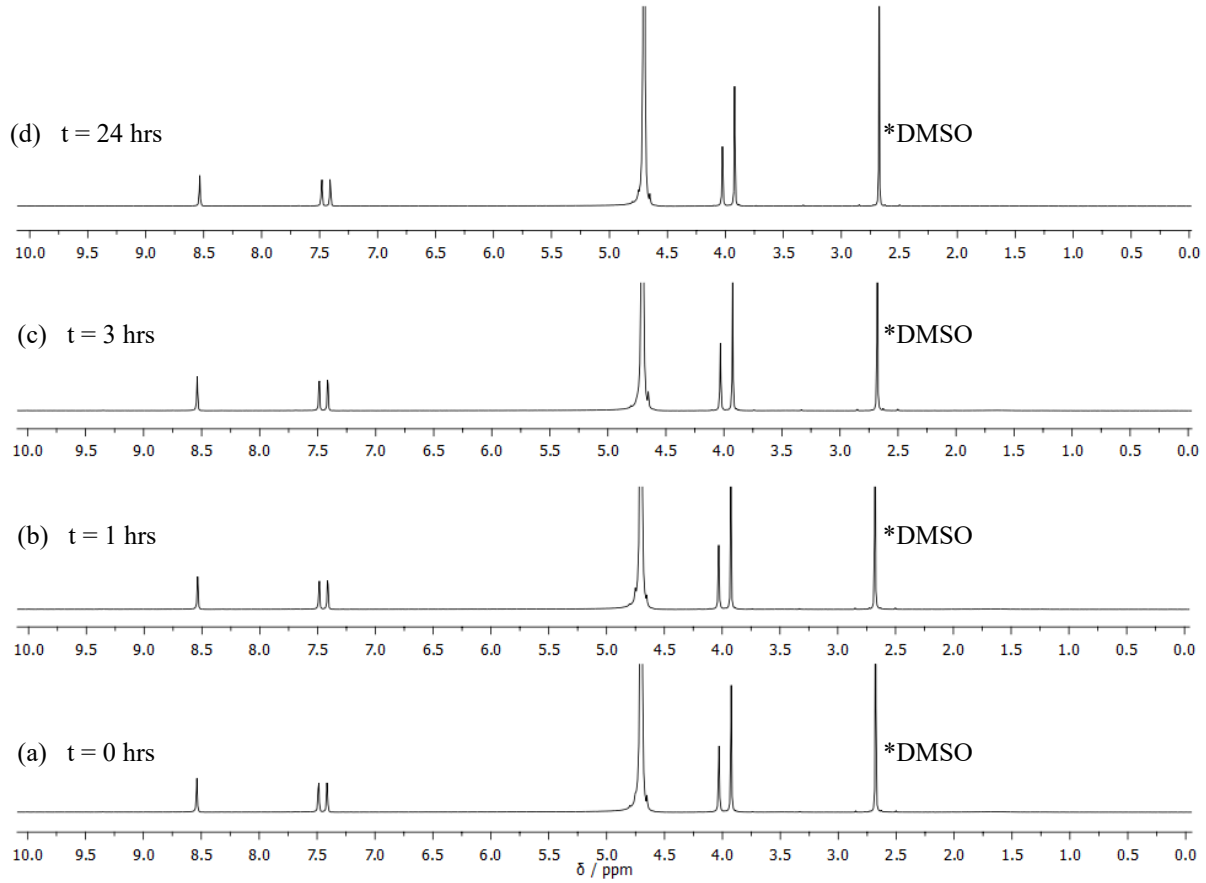

Figure S5. Stability of **Al(III)/MSS** monitored by ^{1}H NMR spectroscopy in D_2O over 24 h, pH* 4.88; Temp. 298.15 K. *DMSO from synthesis.

Table S1. Vertical excitation energies (in eV), oscillator strengths (*f*), wavelengths (λ), and major contributions calculated for **MSS** (I-b-NH and III-c-OH) and **Al(III)/MSS** complex (TD-DFT CAM-B3LYP/6-311++G(d,p), IEFPCM (H_2O)).

Excited State	Energy (eV)	$\lambda_{calc.}$ (nm)	$\lambda_{exp.}$ (nm)	f^a	Major Contributions (%)
					MSS (I-b-NH)
S_1	3.38	367	406	0.36	HOMO–1 → LUMO+1 (43%) HOMO → LUMO (57%)
S_5	4.65	268	295	0.63	HOMO–3 → LUMO+1 (35%) HOMO–2 → LUMO (59%)
S_{11}	5.35	232	249	1.18	HOMO–1 → LUMO+8 (47%) HOMO → LUMO+6 (13%) HOMO → LUMO+7 (17%) HOMO → LUMO+10 (19%)
					MSS (III-c-OH)
S_1	4.19	296	295	0.19	HOMO–1 → LUMO+1 (45%) HOMO → LUMO (55%)
S_3	4.92	252	249	0.75	HOMO–3 → LUMO+1 (35%) HOMO–2 → LUMO (56%)
S_7	5.61	221	-	1.57	HOMO–1 → LUMO+4 (21%) HOMO–1 → LUMO+7 (27%) HOMO → LUMO+5 (30%) HOMO → LUMO+6 (18%)
					Al (III)/MSS

S_1	3.65	340	349	0.01	HOMO–1 → LUMO+1 (35%) HOMO → LUMO (65%)
S_2	3.75	331	-	0.14	HOMO → LUMO+1 (40%) HOMO–3 → LUMO+1 (30%)
S_3	4.59	270	277	0.55	HOMO–2 → LUMO (60%) HOMO–3 → LUMO (60%)
S_4	4.76	260	243	0.24	HOMO–2 → LUMO+1 (40%) HOMO–1 → LUMO+6 (15%)
S_{10}	5.46	227	-	0.93	HOMO–1 → LUMO+7 (29%) HOMO → LUMO+3 (14%) HOMO → LUMO+8 (36%) HOMO–1 → LUMO+3 (15%)
S_{12}	5.58	222	-	0.55	HOMO–1 → LUMO+8 (32%) HOMO → LUMO+6 (15%) HOMO → LUMO+7 (31%)

[a] Results are shown for the region of energy up to 5.61 eV and calculated oscillator strength > 0.01