Electronic Supplementary Material (ESI) for RSC Advances.

Quantum chemical elucidation of the turn-on luminescence mechanism in two new Schiff bases as selective chemosensors of Zn^{2+}: Synthesis, theory and bioimaging applications.

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Supplementary Information

Table S1 Singlet→Singlet absorption transitions for the free sensors**A** and **B** and the coordination compounds.*

	CAM-B3LYP				B3LYP			
System	λ_a	***F***	**Active MOs**	**Assignment**	λ_a	***f***	**Active MOs**	**Assignment**
A	293	0.159	H→L	$\pi-\pi^*$	327	0.105	H→L	$\pi-\pi^*$
	240	0.392	H-1→L	$\pi-\pi^*$	258	0.344	H-1→L	$\pi-\pi^*$
A/Ni^{2+}	334	0.128	H→L	$\pi-\pi^*$	379	0.036	H→L	$\pi-\pi^*$
	255	0.172	H-1→L	$\pi-\pi^*$	369	0.111	H-1→L	$\pi-\pi^*$
A/Zn^{2+}	319	0.173	H→L	$\pi-\pi^*$	354	0.122	H→L	$\pi-\pi^*$
	246	0.279	H-1→L	$\pi-\pi^*$	303	0.037	H-1→L	$\pi-\pi^*$
B	278	0.182	H→L	$\pi-\pi^*$	303	0.126	H→L	$\pi-\pi^*$
	232	0.341	H-1→L	$\pi-\pi^*$	242	0.348	H-1→L	$\pi-\pi^*$
B/Ni^{2+}	323	0.159	H→L	$\pi-\pi^*$	368	0.057	H→L	$\pi-\pi^*$
	250	0.121	H-1→L	$\pi-\pi^*$	300	0.008	H-1→L	$\pi-\pi^*$
B/Zn^{2+}	306	0.264	H→L	$\pi-\pi^*$	336	0.138	H→L	$\pi-\pi^*$
	241	0.185	H-1→L	$\pi-\pi^*$	284	0.022	H-1→L	$\pi-\pi^*$

*λ_a: calculated absorption wavelength in nm
f: oscillator strength

Table S2 Singlet→Singlet emission transitions for the free sensors **A** and **B** and the coordination compounds.*

	CAM-B3LYP					B3LYP				
System	λ_e	***f***	k_{rad}	**τ**	**Assignment**	λ_e	***f***	k_{rad}	**τ**	**Assignment**
A	391	0.020	$2.9*10^8$	$3.4*10^{-9}$	π–π*	510	0.009	$4.2*10^8$	$2.3*10^{-9}$	π–π*
A/Ni²⁺	377	0.006	$4.7*10^7$	$2.1*10^{-8}$	dNi-π	486	0.002	$2.0*10^6$	$5.0*10^{-7}$	dNi-π
A/Zn²⁺	455	0.063	$2.0*10^7$	$3.2*10^{-8}$	π–π*	498	0.055	$2.0*10^7$	$5.1*10^{-9}$	π–π*
B	539	0.002	$2.5*10^8$	$4.0*10^{-9}$	π–π*	460	0.004	$4.3*10^8$	$2.3*10^{-9}$	π–π*
B/Ni²⁺	351	0.009	$1.2*10^7$	$8.1*10^{-8}$	dNi-π	441	0.003	$1.7*10^8$	$6.0*10^{-9}$	dNi-π
B/Zn²⁺	373	0.026	$1.0*10^8$	$9.6*10^{-9}$	π–π*	494	0.025	$1.0*10^7$	$1.1*10^{-8}$	π–π*

*λ_e:calculated emission wavelength in nm
f:oscillator strength
k_{rad}: emission radiative rate in s^{-1}
t: emission radiative lifetime in s.

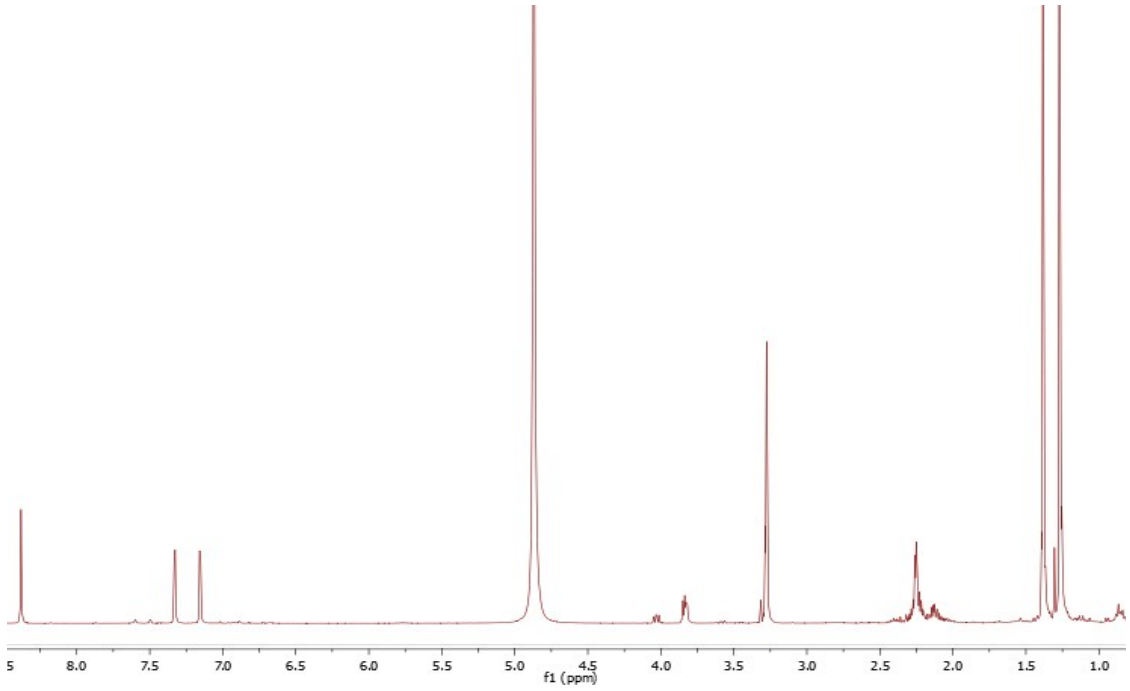

Figure S1. ^{1}H-NMR (400 MHz, CD_3OD, 298 K) spectrum of compound **A**.

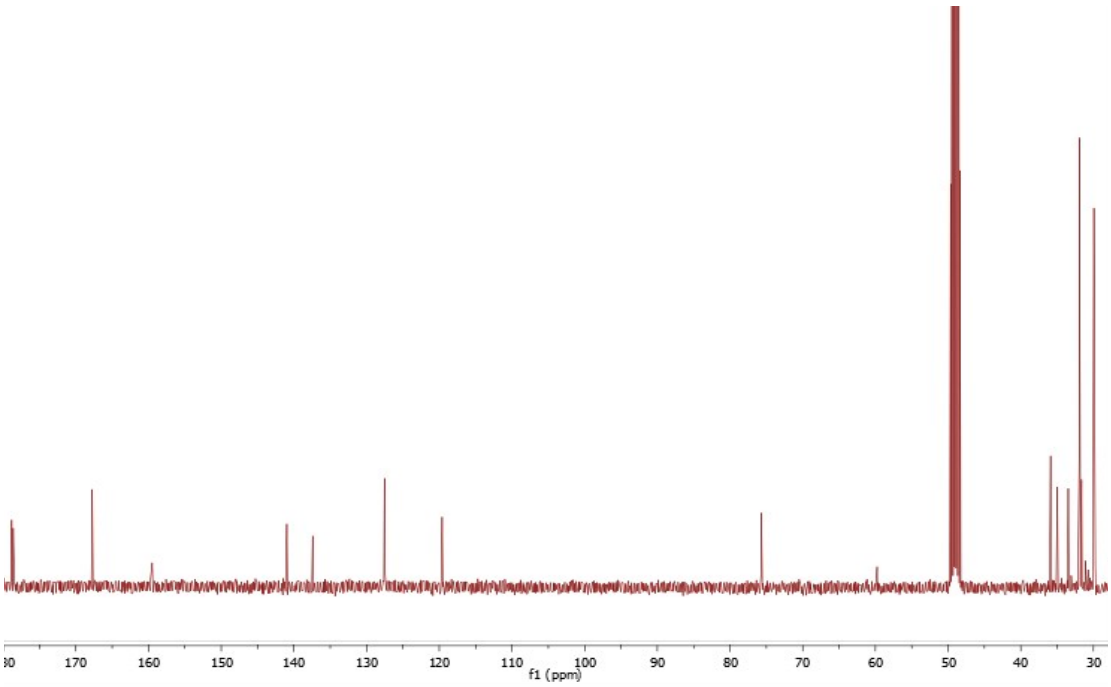

Figure S2. ^{13}C-NMR (400 MHz, CD_3OD, 298 K) spectrum of compound **A**.

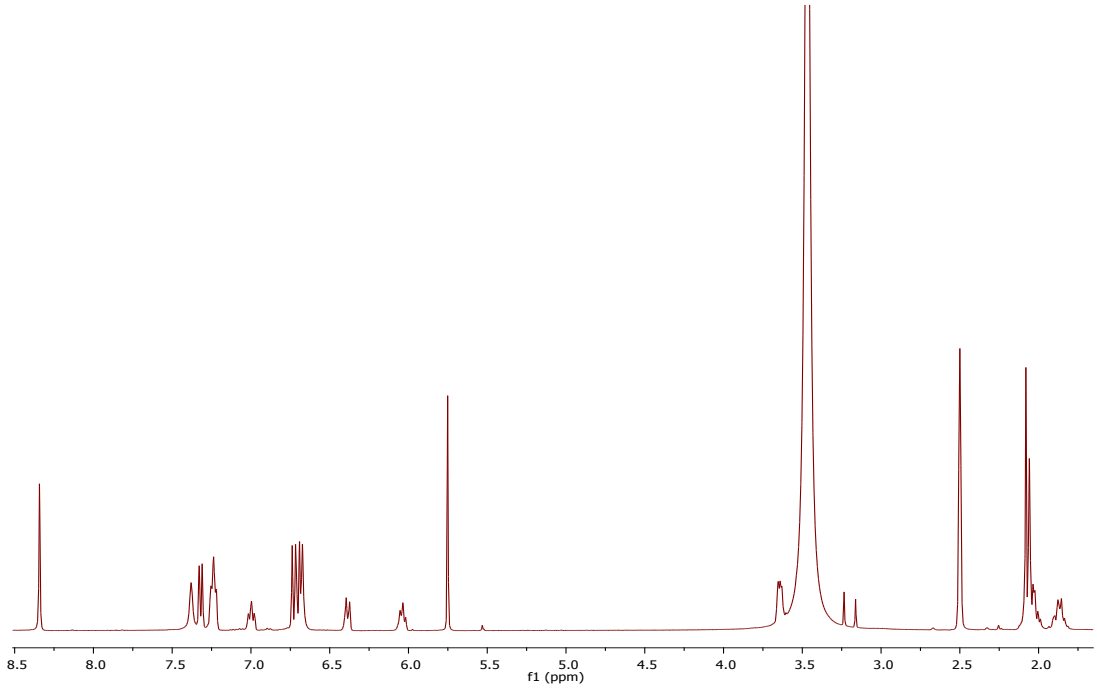

Figure S3. ^{1}H-NMR (400 MHz, CD_3OD, 298 K) spectrum of compound **B**.

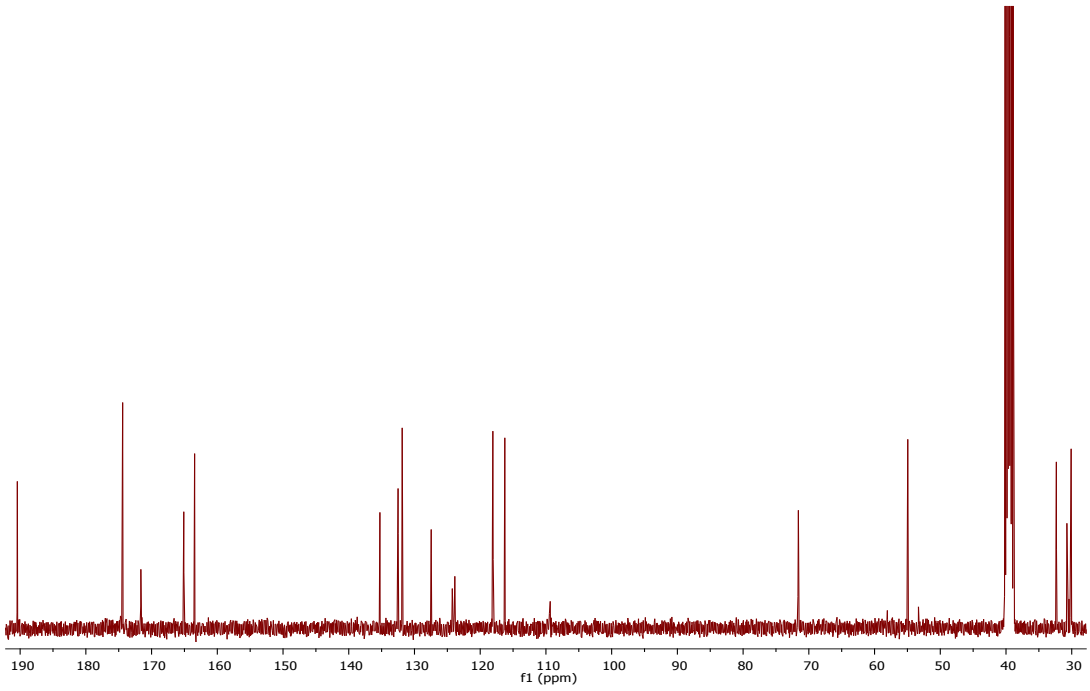

Figure S4. ^{13}C-NMR (400 MHz, CD_3OD, 298 K) spectrum of compound **B**

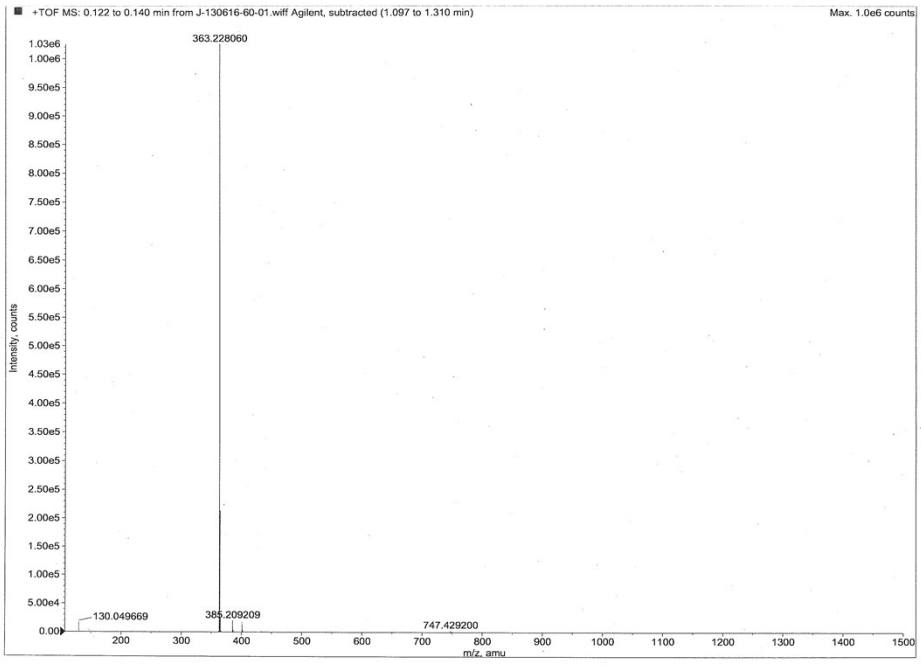

Figure S5. Mass spectrum of compound **A**.

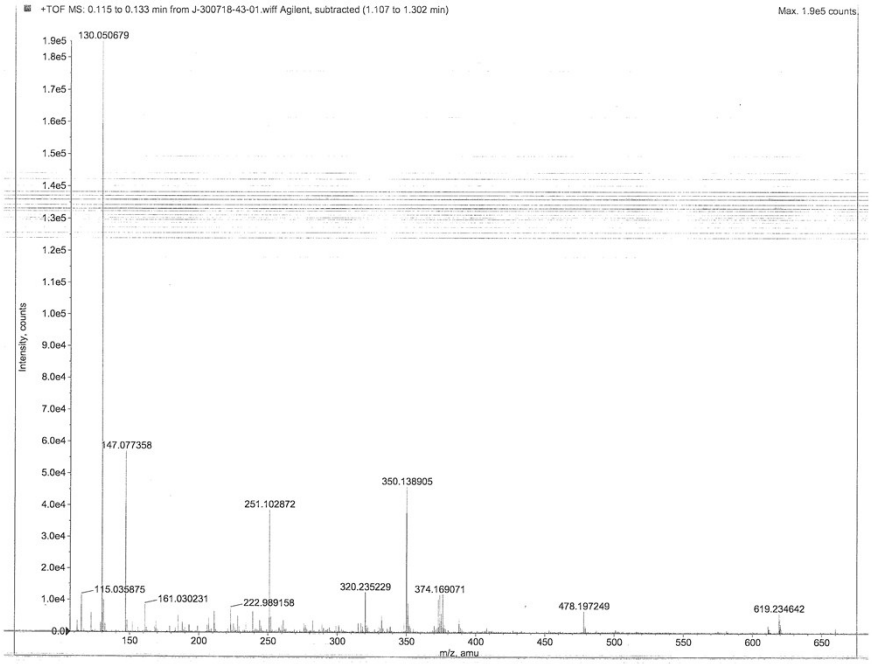

Figure S6. Mass spectrum of compound **B**.