

## **Supplementary Information**

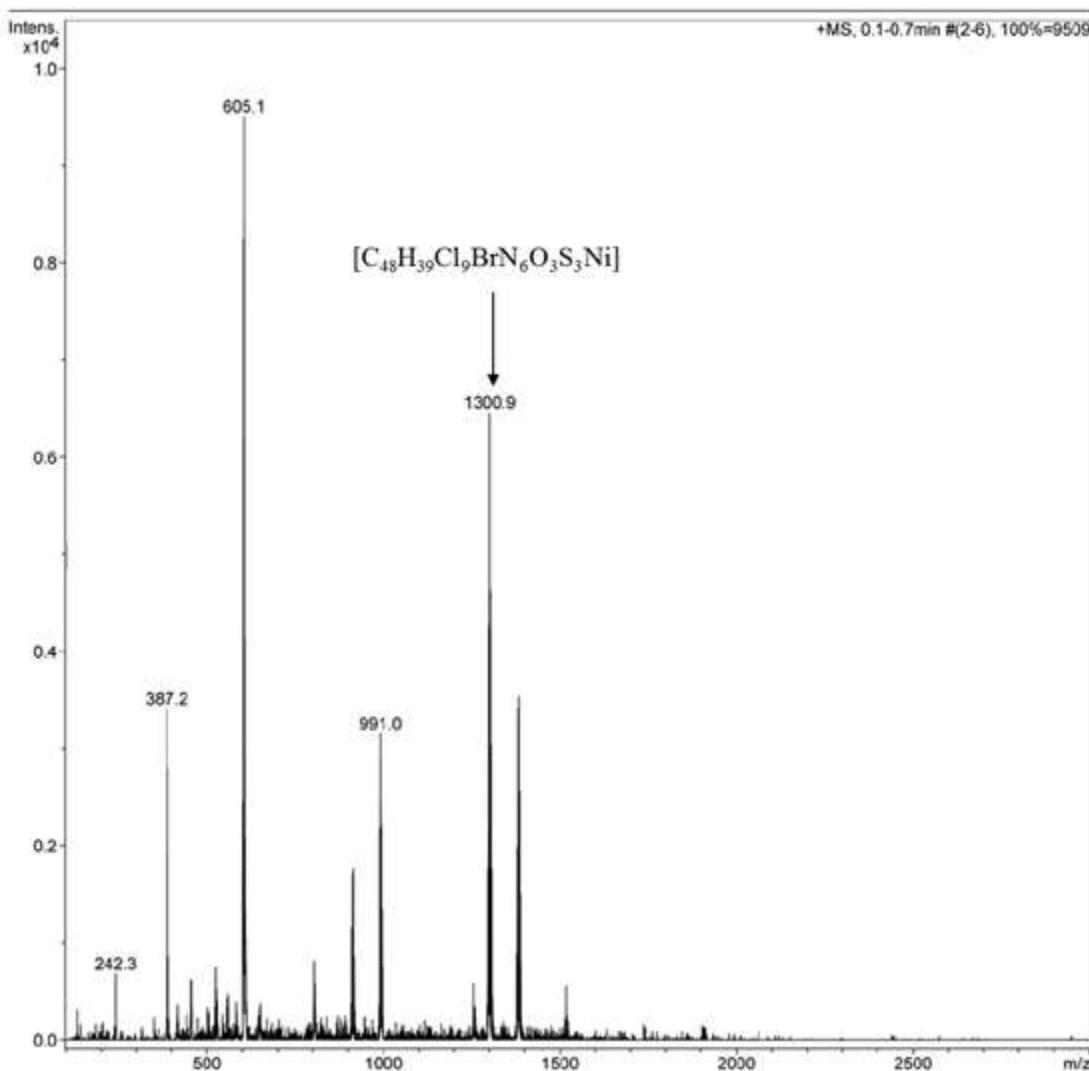
Synthesis, characterization and cytotoxic activity of tioconazole coordination compounds with nickel(II), palladium(II) and platinum(II)

Carmela Crisóstomo-Lucas<sup>1</sup>, Rubí Navarro-PeñaLoza<sup>1</sup>, Naytzé Ortiz-Pastrana<sup>1,2</sup>, Francisco Sánchez-Bartéz<sup>1,3</sup>, Isabel Gracia-Mora<sup>1,3</sup>, Norah Barba-Behrens<sup>1\*</sup>

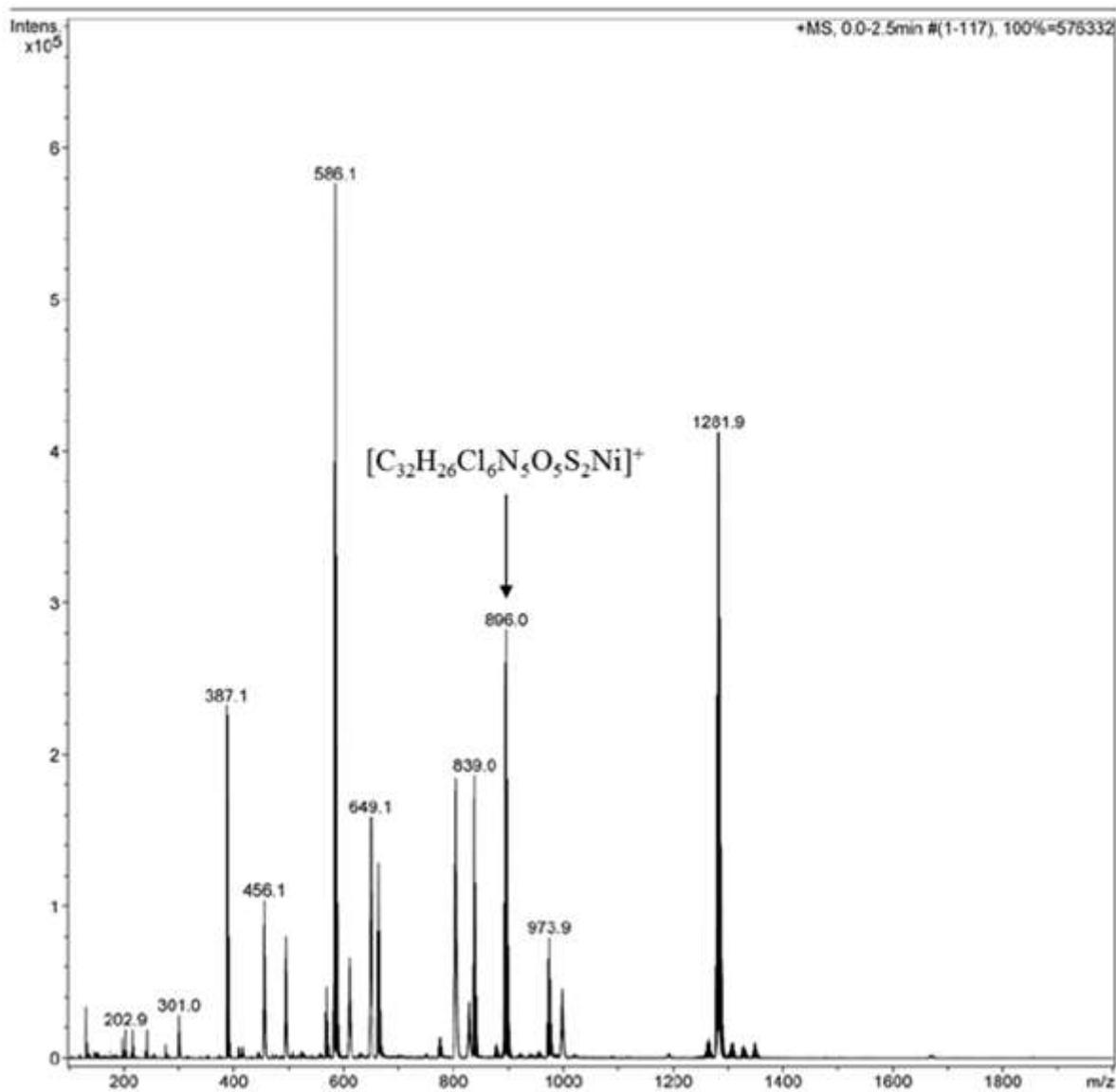
<sup>1</sup>Departamento de Química Inorgánica, Facultad de Química, Universidad Nacional Autónoma de México, Ciudad Universitaria, Coyoacán, 04510, Ciudad de México, México.

<sup>2</sup>Departamento de Química, Cinvestav, AP 14-740, 07000, Ciudad de México, México

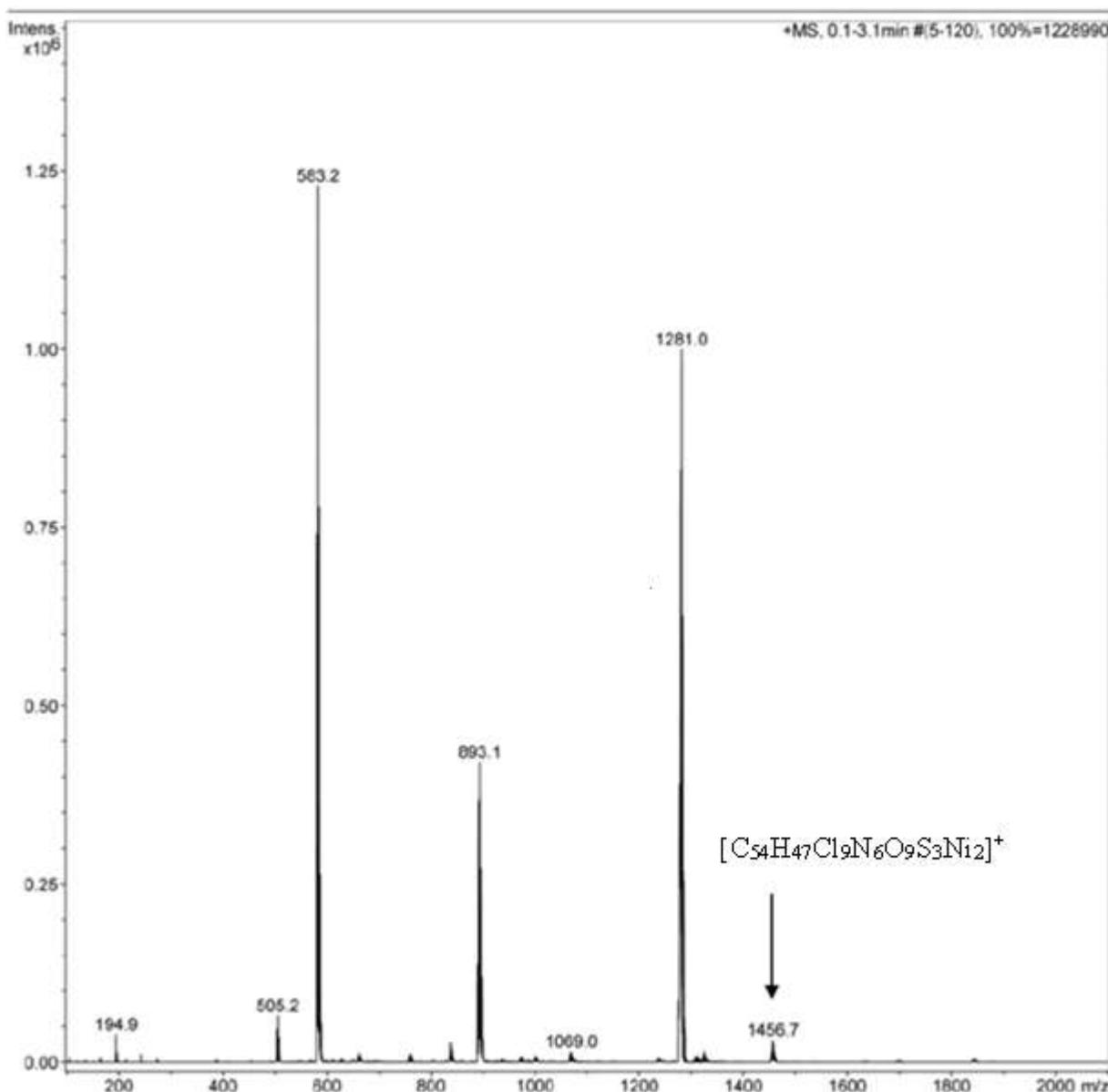
<sup>3</sup>Unidad de Investigación Preclínica (UNIPREC), Facultad de Química, Universidad Nacional Autónoma de México, Ciudad de México, México



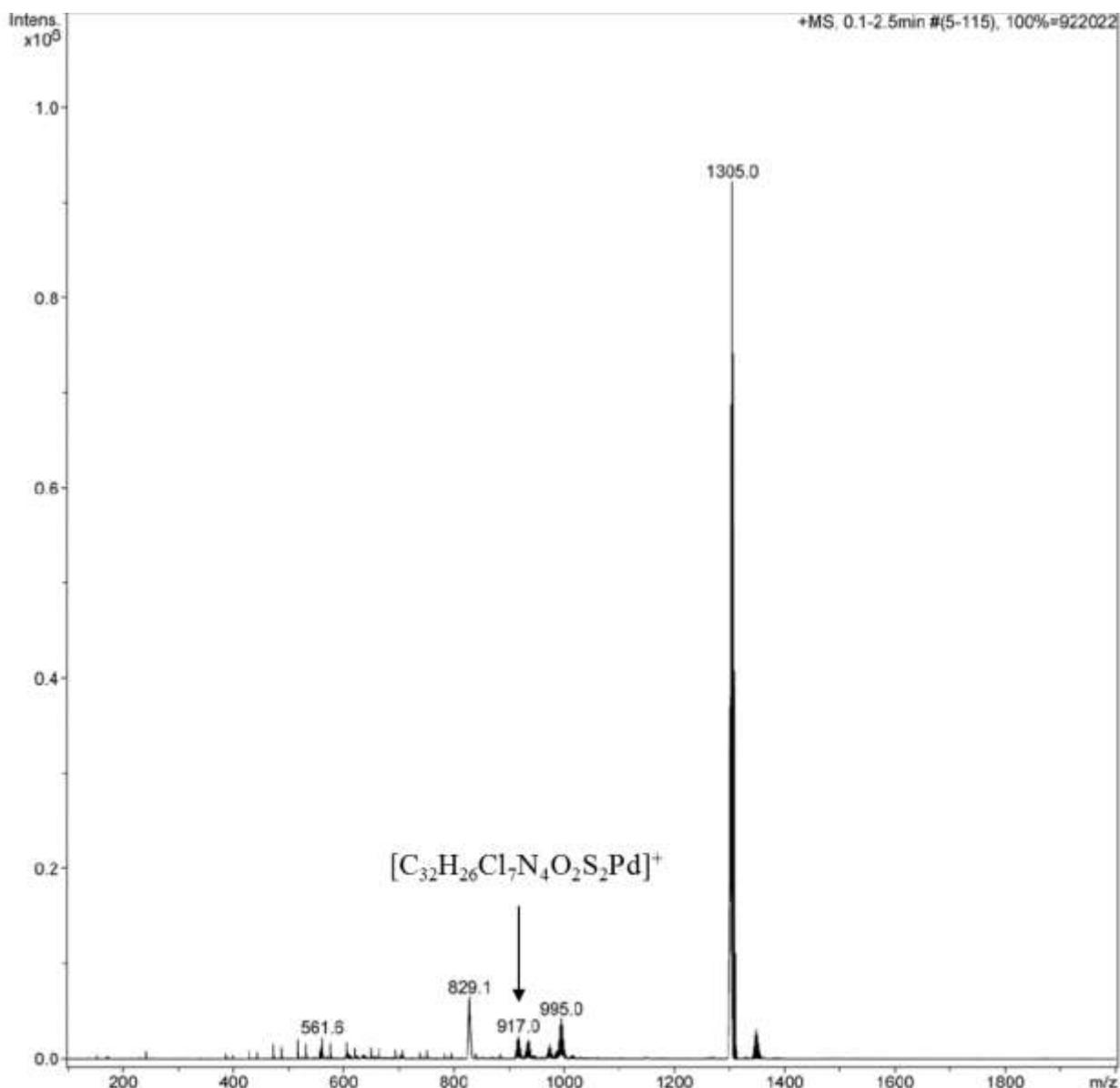
**Figure S1.** MS-ESI<sup>+</sup> spectrum of  $[Ni(tcnz)_3Br_2(H_2O)]$  **1**.



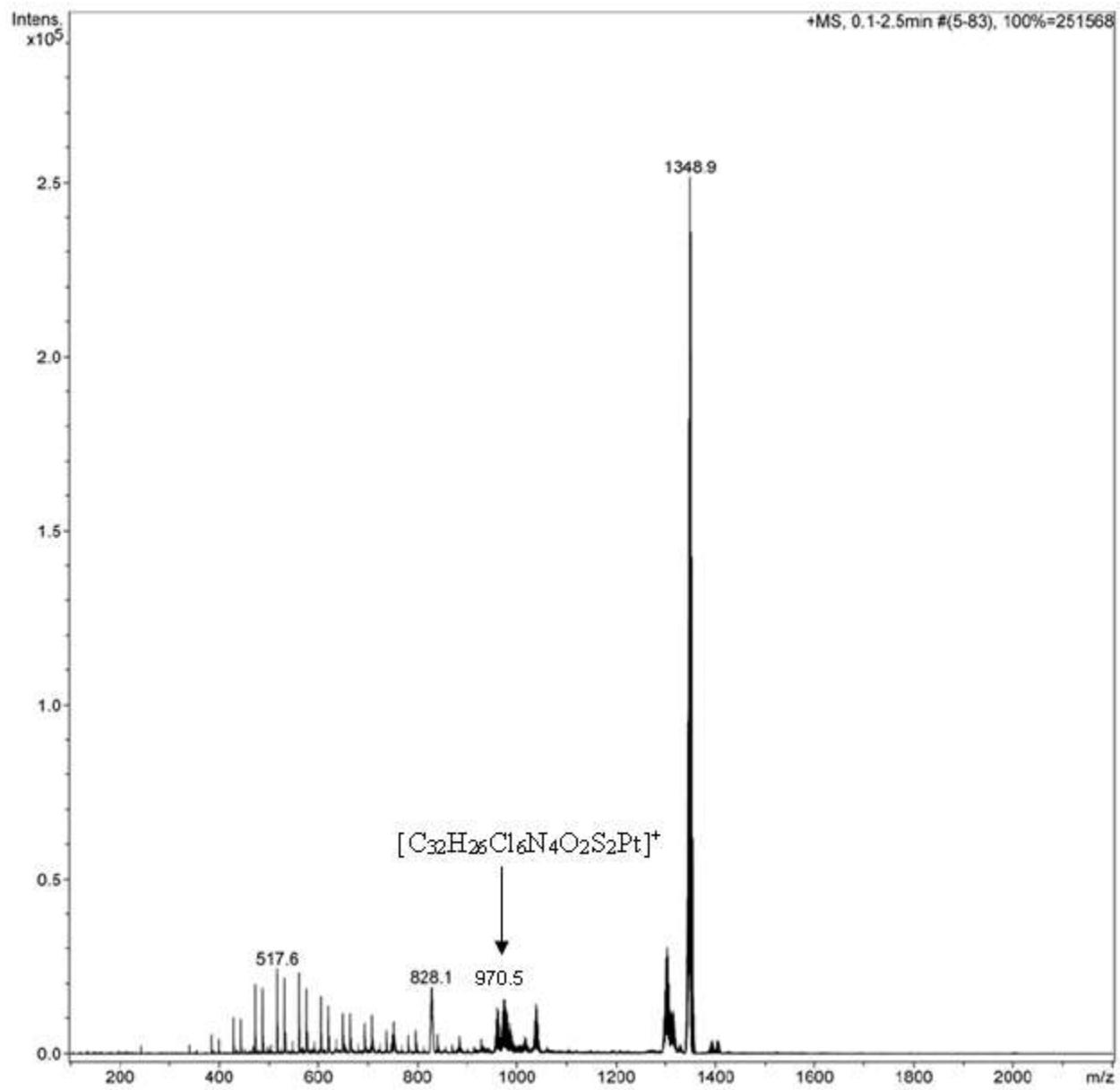
**Figure S2.** MS-ESI<sup>+</sup> spectrum of  $[Ni(tcnz)_2(NO_3)_2] \cdot H_2O$  **2**.



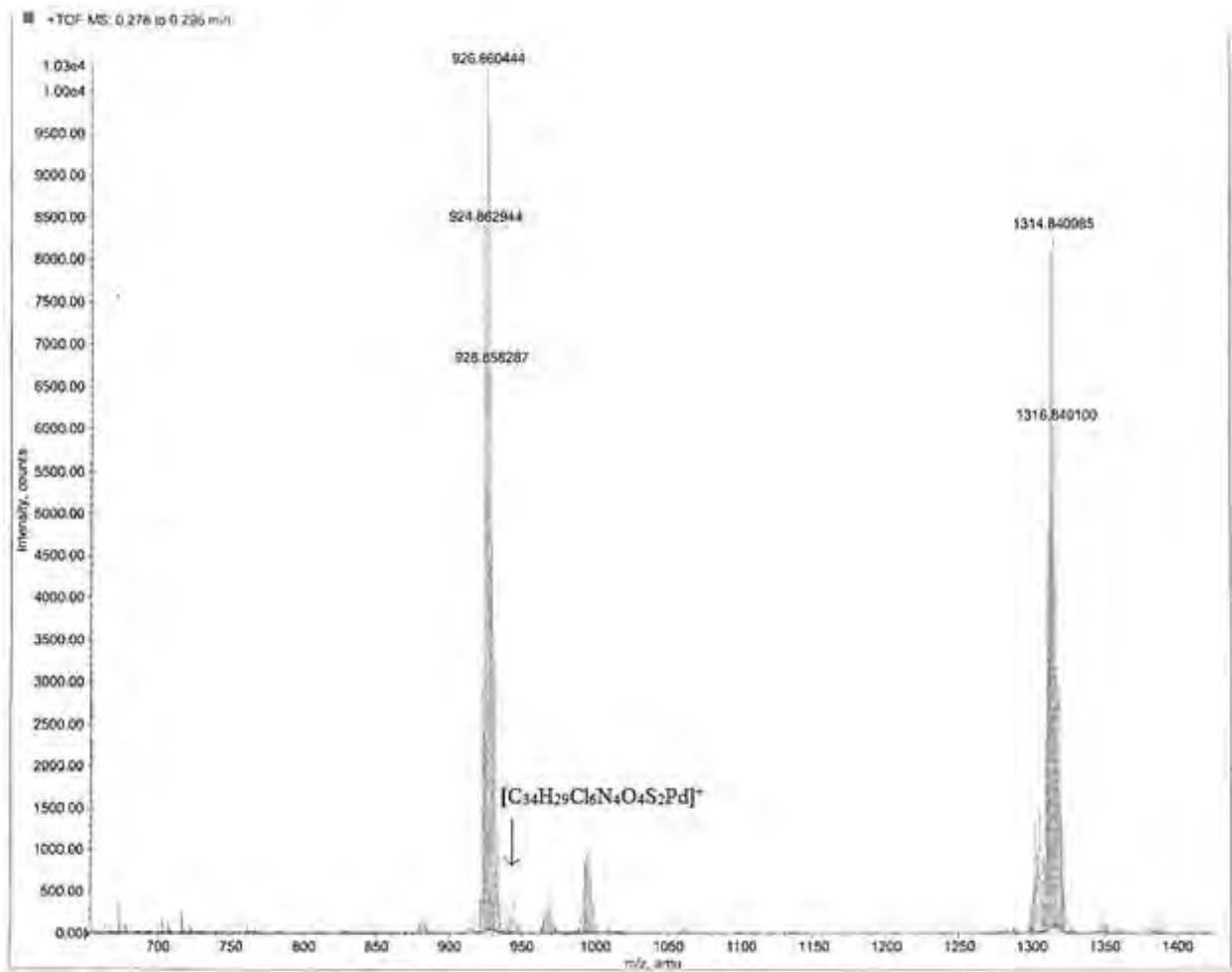
**Figure S3.** MS-ESI<sup>+</sup> spectrum  $[Ni(tcnz)_2(OAc)_2] \cdot 3H_2O$  **3**.



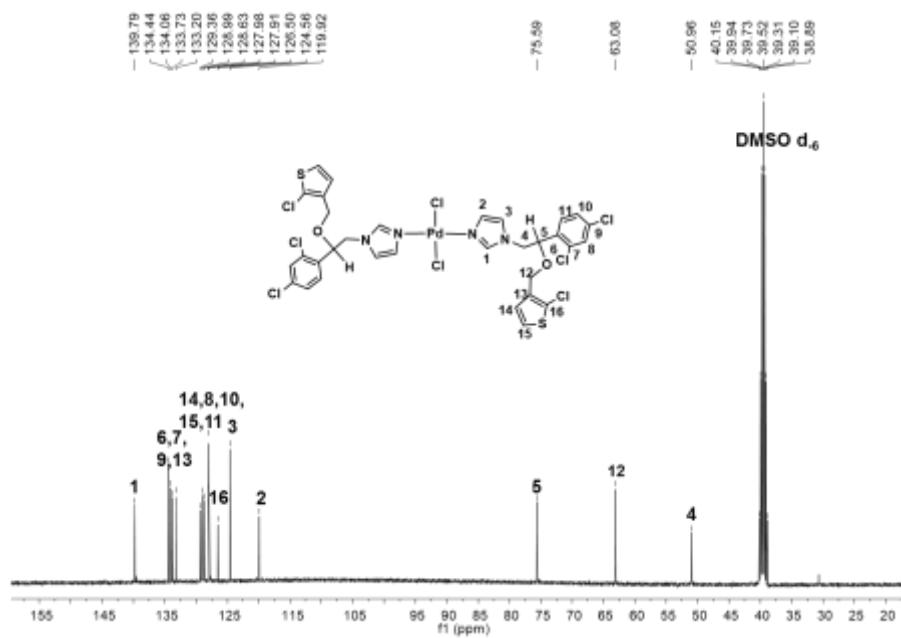
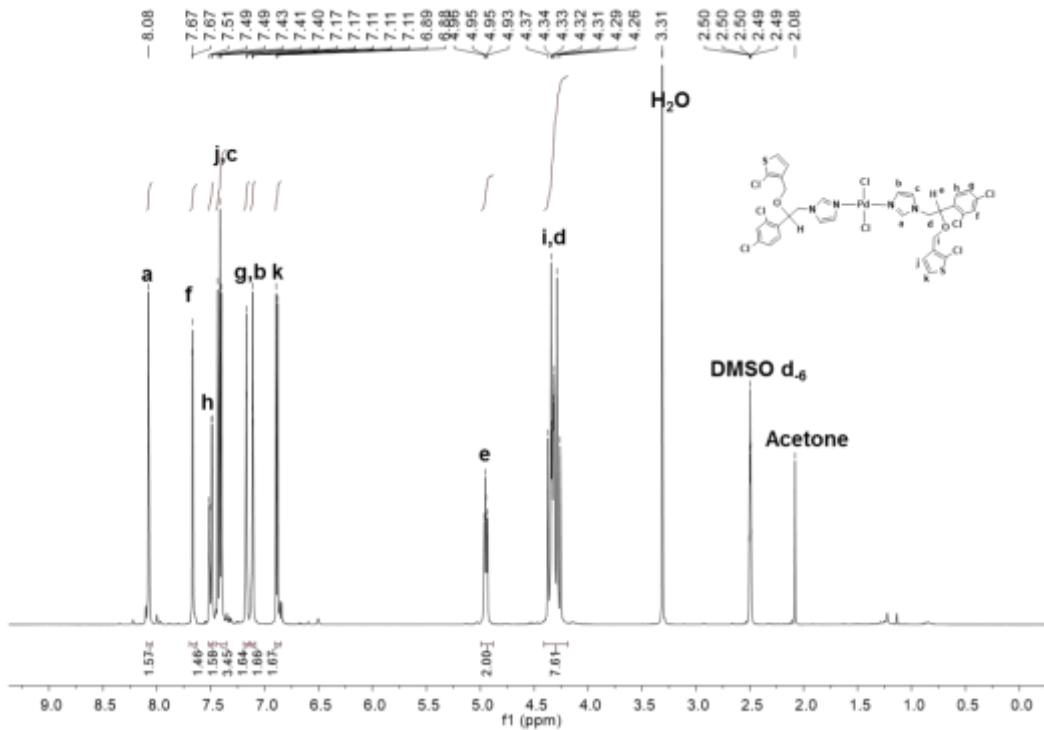
**Figure S4.** MS-ESI<sup>+</sup> spectrum of [Pd(tcnz)<sub>2</sub>Cl<sub>2</sub>] **6**.

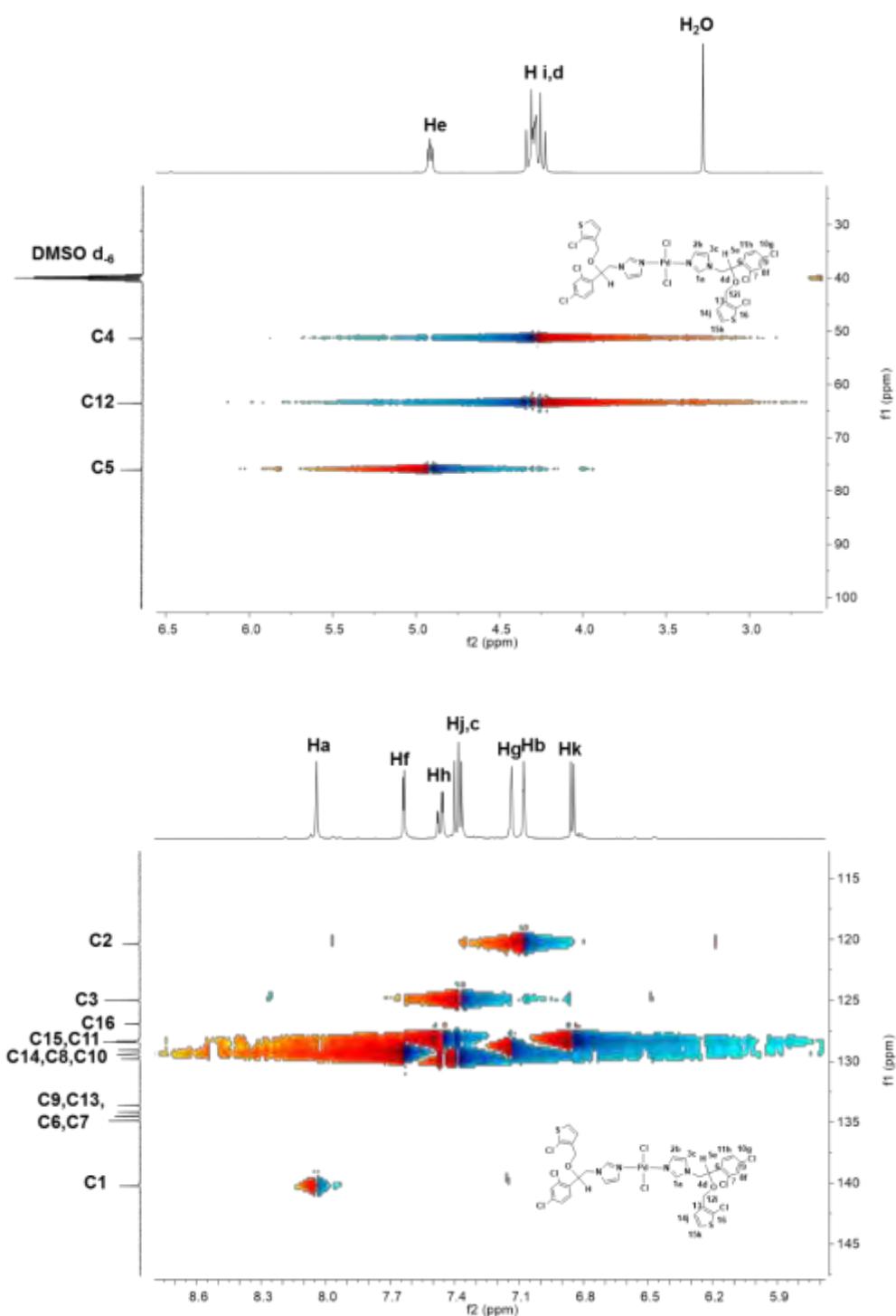


**Figure S5.** MS-ESI<sup>+</sup> spectrum of  $[Pt(tcnz)_2Cl_2] \cdot 2H_2O$  **7**.

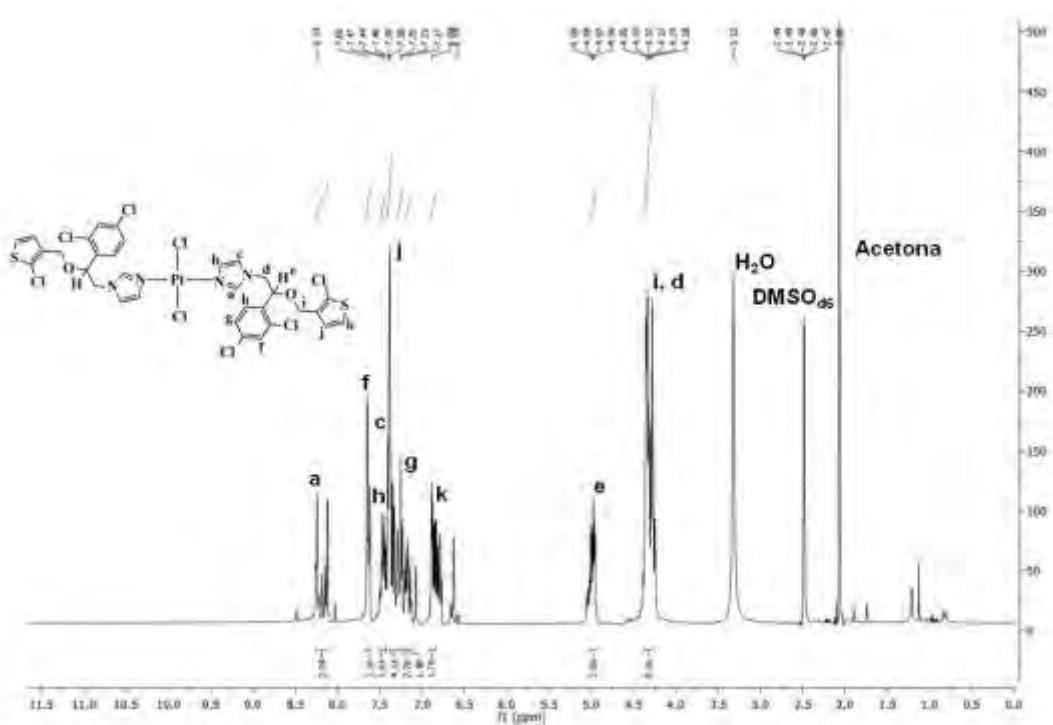


**Figure S6.** MS-TOF<sup>+</sup> spectrum of [Pd(tcnz)<sub>2</sub>(OAc)<sub>2</sub>] **8**.

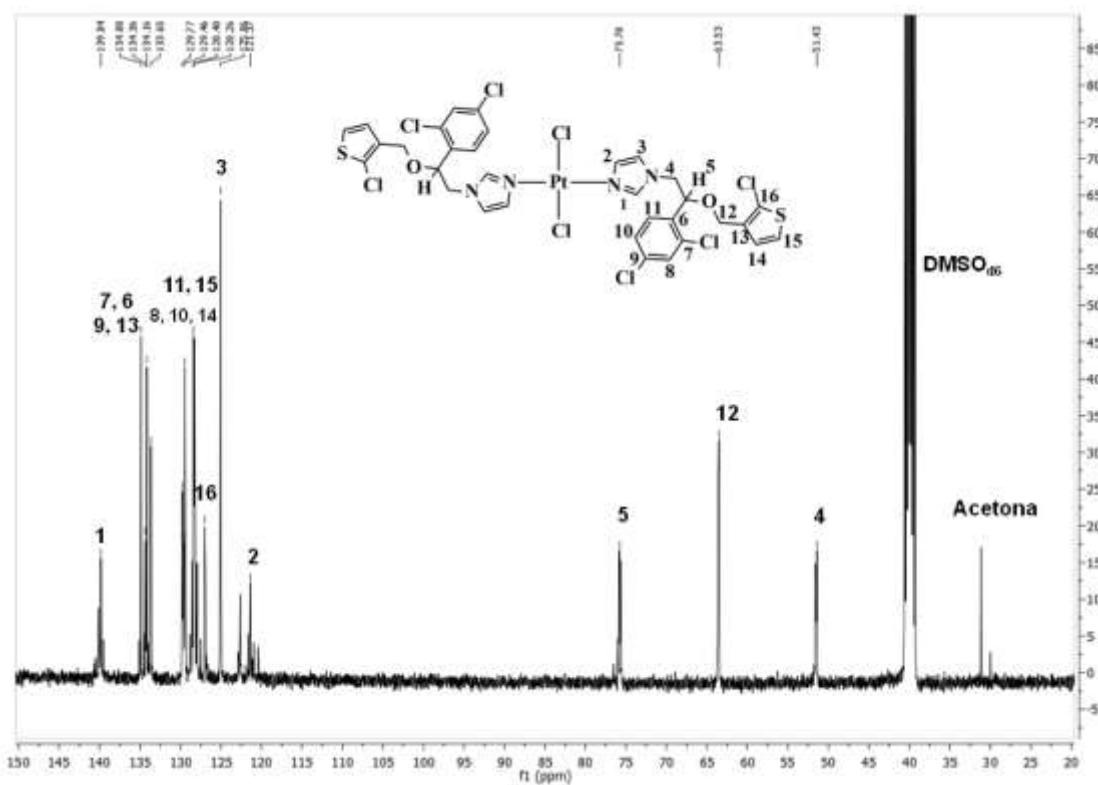




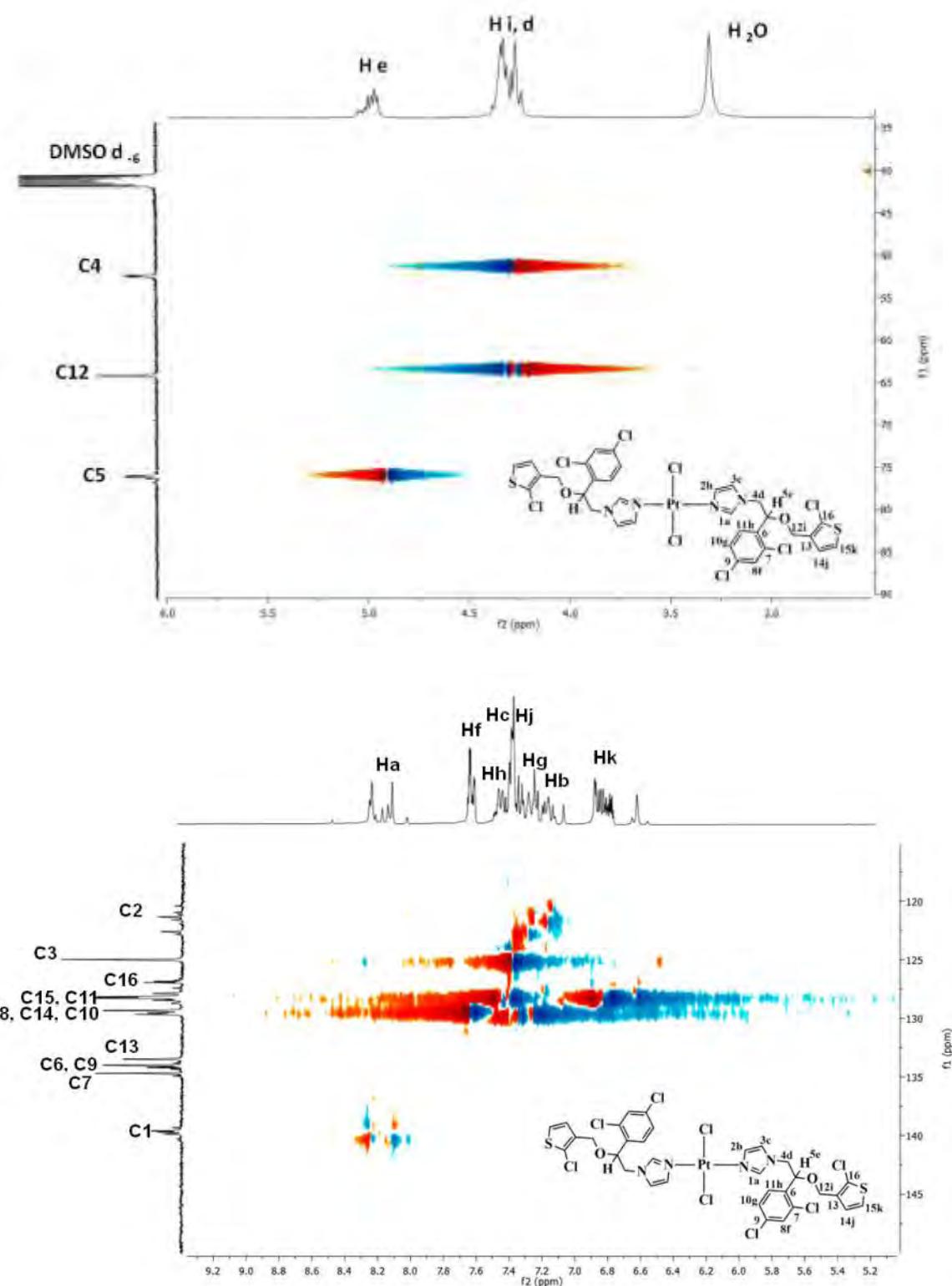
**Figure S9.** HSQC NMR spectra of  $[\text{Pd}(\text{tcnz})_2\text{Cl}_2]$  **6** in  $\text{DMSO}-\text{d}_6$ .



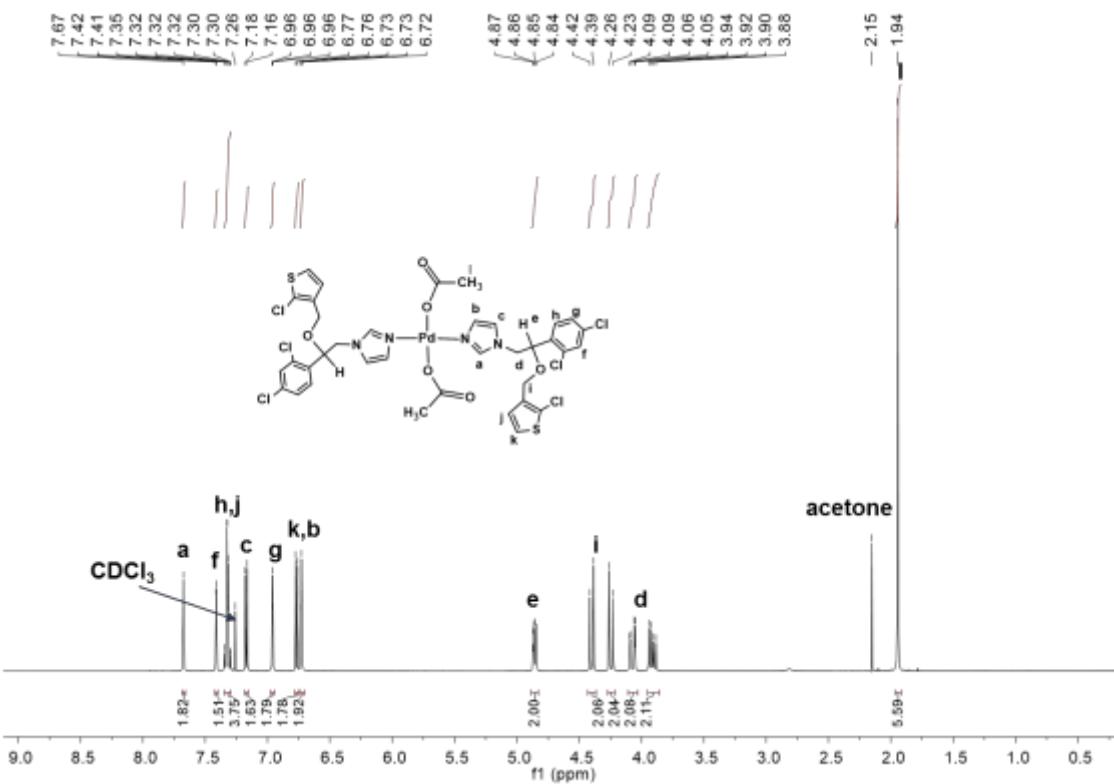
**Figure S10.**  $^1\text{H}$  NMR spectrum of  $[\text{Pt}(\text{tcnz})_2\text{Cl}_2]$  **7** in  $\text{CDCl}_3$ .



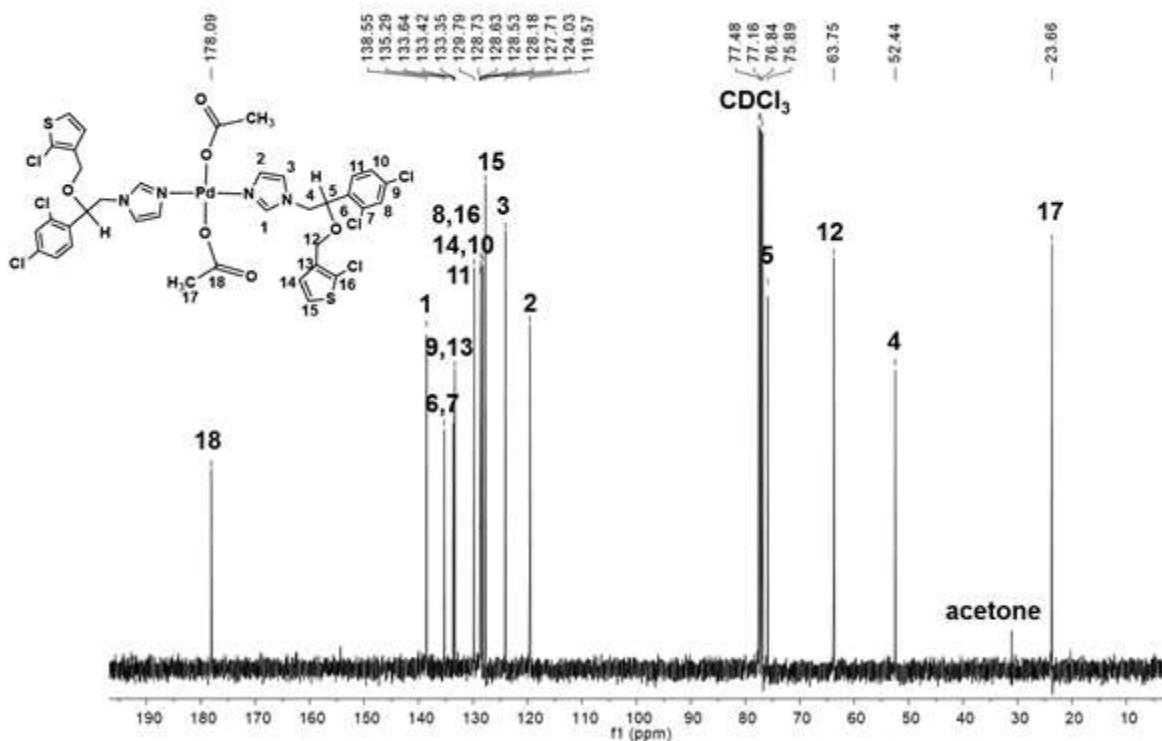
**Figure S11.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of  $[\text{Pt}(\text{tcnz})_2\text{Cl}_2]$  **7** in  $\text{CDCl}_3$ .



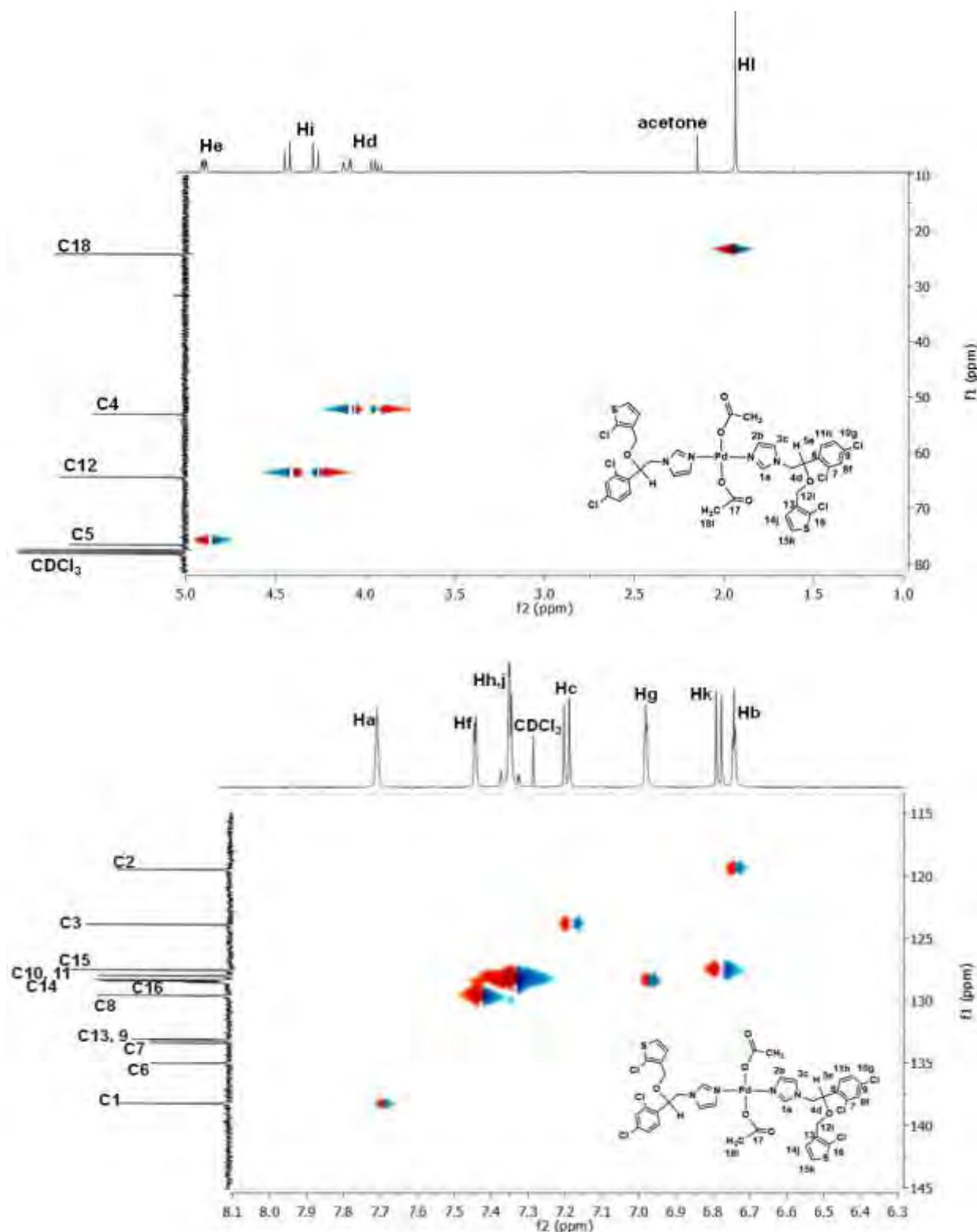
**Figure S12.** HSQC NMR spectra of  $[\text{Pt}(\text{tcnz})_2\text{Cl}_2]$  **7** in  $\text{CDCl}_3$ .



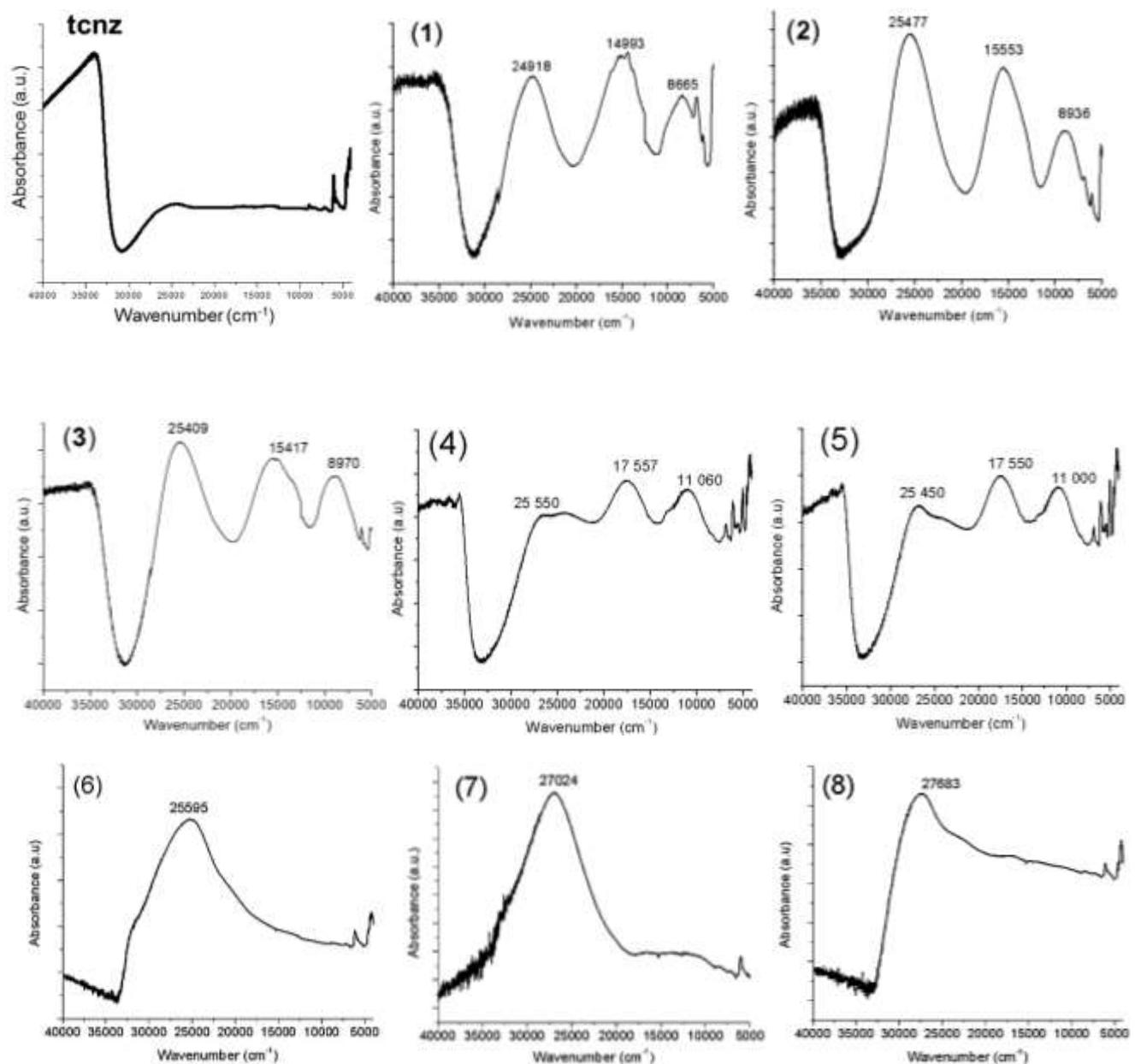
**Figure S13.**  $^1\text{H}$  NMR spectrum of  $[\text{Pd}(\text{tcnz})_2(\text{OAc})_2]$  **8** in  $\text{CDCl}_3$ .



**Figure S14.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of  $[\text{Pd}(\text{tcnz})_2(\text{OAc})_2]$  **8** in  $\text{CDCl}_3$ .



**Figure S15.** HSQC NMR spectra of  $[\text{Pd}(\text{tcnz})_2(\text{OAc})_2]$  **8** in  $\text{CDCl}_3$ .



**Figure S16.** Solid state UV-Vis-NIR  $\nu(\text{cm}^{-1})$  of tioconazole compounds of  $\text{Ni}^{\text{II}}$ ,  $\text{Pd}^{\text{II}}$  and  $\text{Pt}^{\text{II}}$ .