

Supplementary Materials:

# Coordination Properties of the Fungal Metabolite Harzianic Acid toward Toxic Heavy Metals

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**Figure S1.** Mass spectrum ESIMS QTOF obtained by LC-MS analysis in ESI positive mode of a solution  $1.0 \times 10^{-3}$  M of harzianic acid and  $1.0 \times 10^{-3}$  M of  $\text{Cd}(\text{ClO}_4)_2$  in MeOH/H<sub>2</sub>O 50:50 (*w/w*).

**Figure S2.** Mass spectrum ESIMS QTOF obtained by LC-MS analysis in ESI positive mode of a solution  $1.0 \times 10^{-3}$  M of harzianic acid and  $1.0 \times 10^{-3}$  M of  $\text{CoCl}_2$  in MeOH/H<sub>2</sub>O 50:50 (*w/w*).

**Figure S3.** Mass spectrum ESIMS QTOF obtained by LC-MS analysis in ESI positive mode of a solution  $1.0 \times 10^{-3}$  M of harzianic acid and  $1.0 \times 10^{-3}$  M of  $\text{NiCl}_2$  in MeOH/H<sub>2</sub>O 50:50 (*w/w*).

**Figure S4.** Mass spectrum ESIMS QTOF obtained by LC-MS analysis in ESI positive mode of a solution  $1.0 \times 10^{-3}$  M of harzianic acid and  $1.0 \times 10^{-3}$  M of  $\text{Pb}(\text{ClO}_4)_2$  in MeOH/H<sub>2</sub>O 50:50 (*w/w*).

**Figure S5.** <sup>1</sup>H NMR spectra of harzianic acid (HA) (down),  $\text{Cd}(\text{ClO}_4)_2$  : HA (middle) and  $\text{Pb}(\text{ClO}_4)_2$  : HA (up) recorded in CD<sub>3</sub>OD/D<sub>2</sub>O (50:50 *w/w*) at 400 MHz. Solvent peaks are removed.

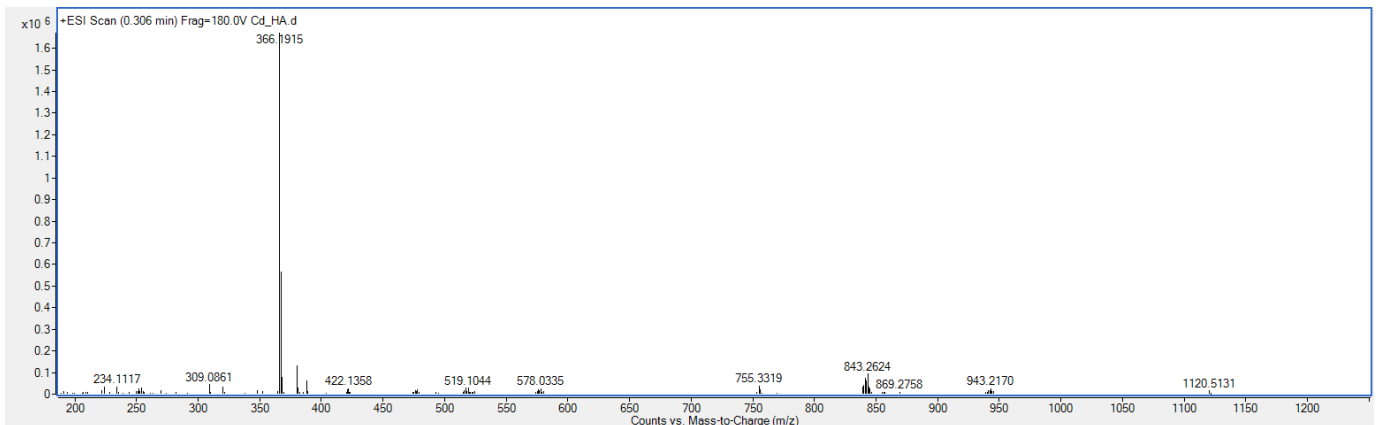
**Figure S6.** Solid-state FT-IR spectrum of harzianic acid.

**Figure S7.** Solid-state FT-IR spectrum of Cd (II)/harzianic acid complex.

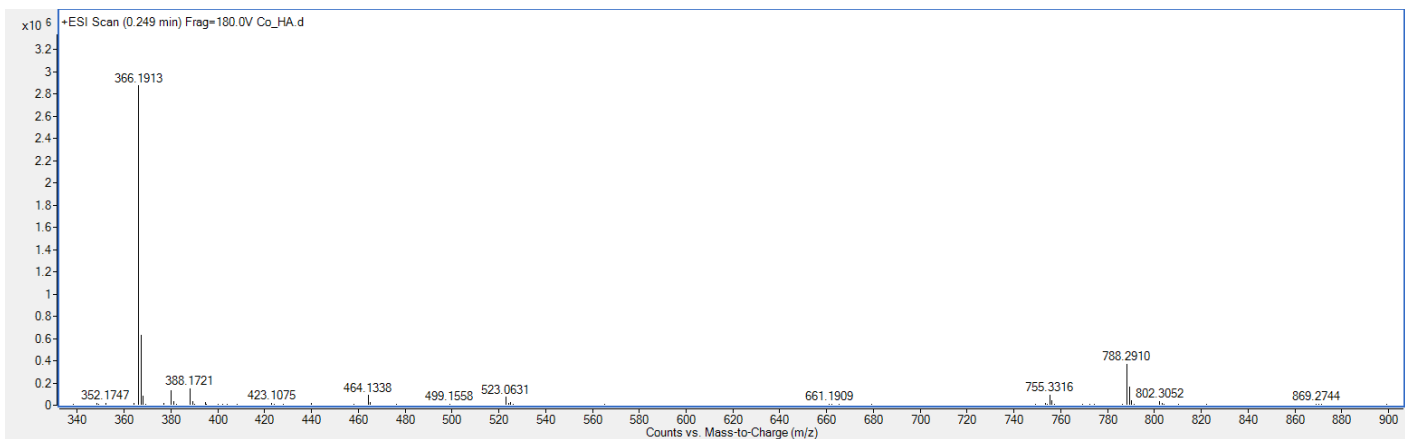
**Figure S8.** Solid-state FT-IR spectrum of Co (II)/harzianic acid complex.

**Figure S9.** Solid-state FT-IR spectrum of Ni (II)/harzianic acid complex.

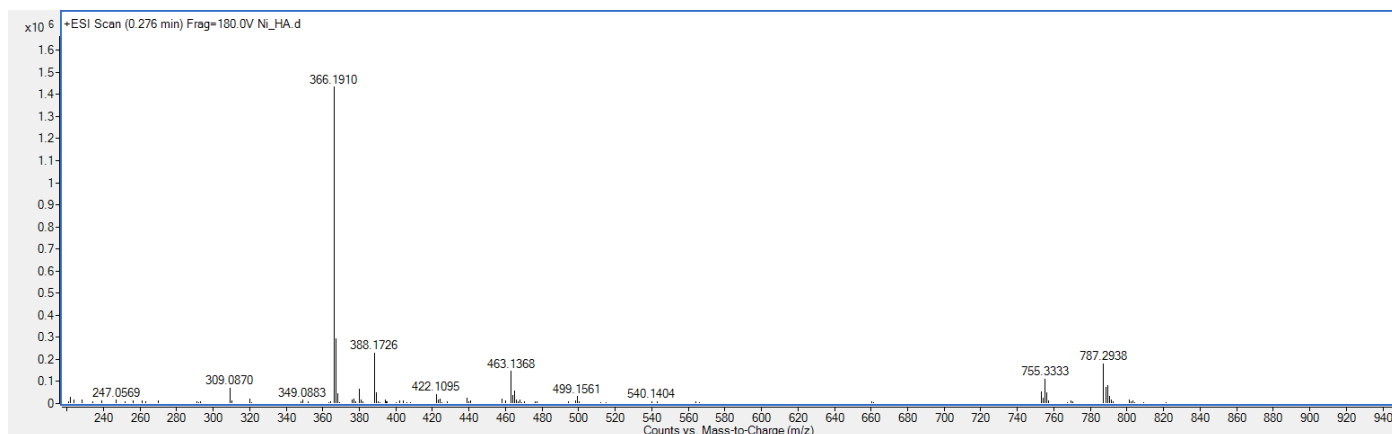
**Figure S10.** Solid-state FT-IR spectrum of Pb (II)/harzianic acid complex.



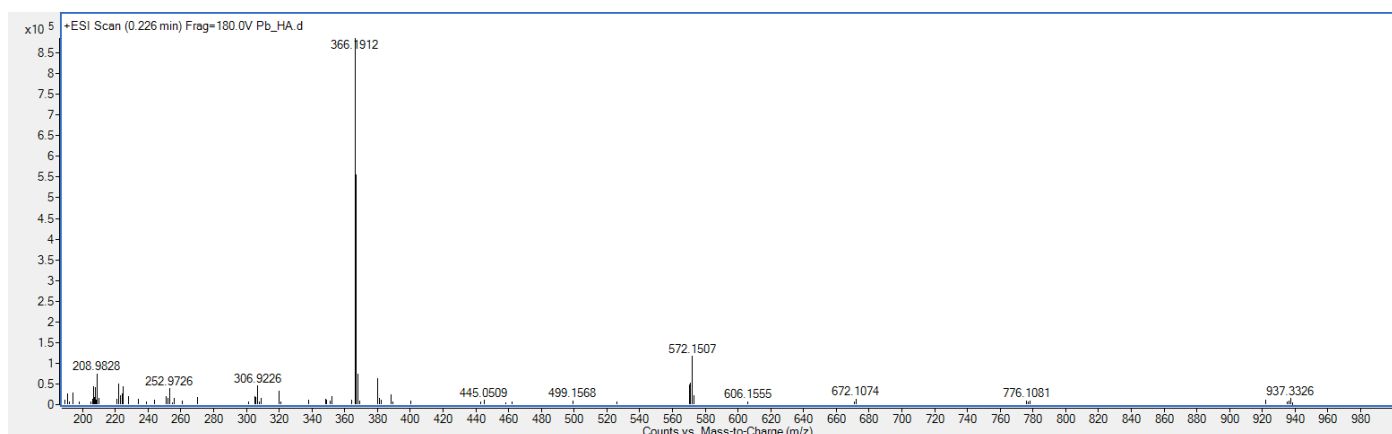
**Figure S1.** Mass spectrum ESIMS QTOF obtained by LC-MS analysis in ESI positive mode of a solution  $1.0 \times 10^{-3}$  M of harzianic acid and  $1.0 \times 10^{-3}$  M of  $\text{Cd}(\text{ClO}_4)_2$  in  $\text{MeOH}/\text{H}_2\text{O}$  50:50 (*w/w*).



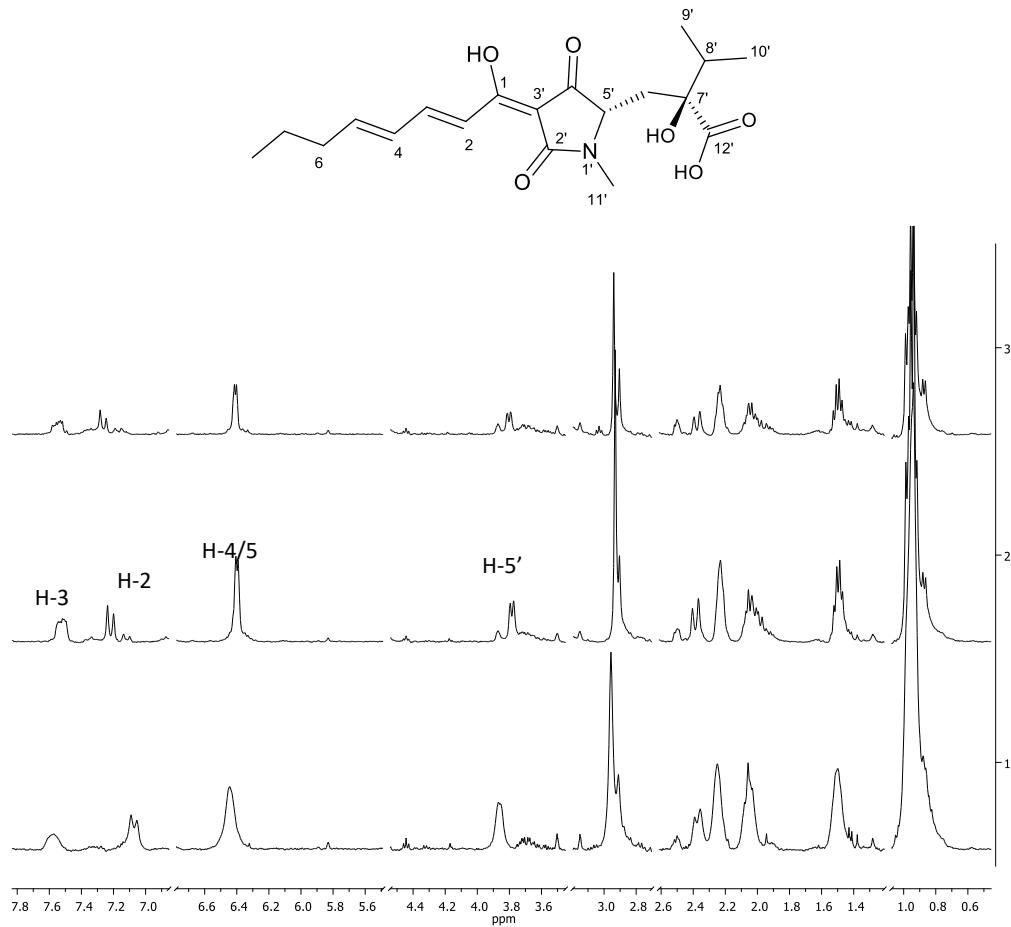
**Figure S2.** Mass spectrum ESIMS QTOF obtained by LC-MS analysis in ESI positive mode of a solution  $1.0 \times 10^{-3}$  M of harzianic acid and  $1.0 \times 10^{-3}$  M of  $\text{CoCl}_2$  in  $\text{MeOH}/\text{H}_2\text{O}$  50:50 (*w/w*).



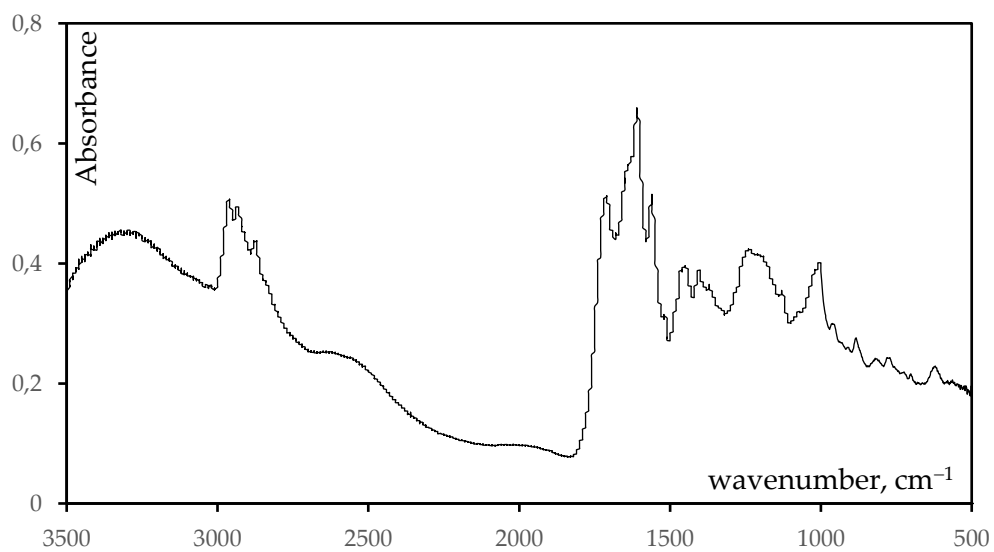
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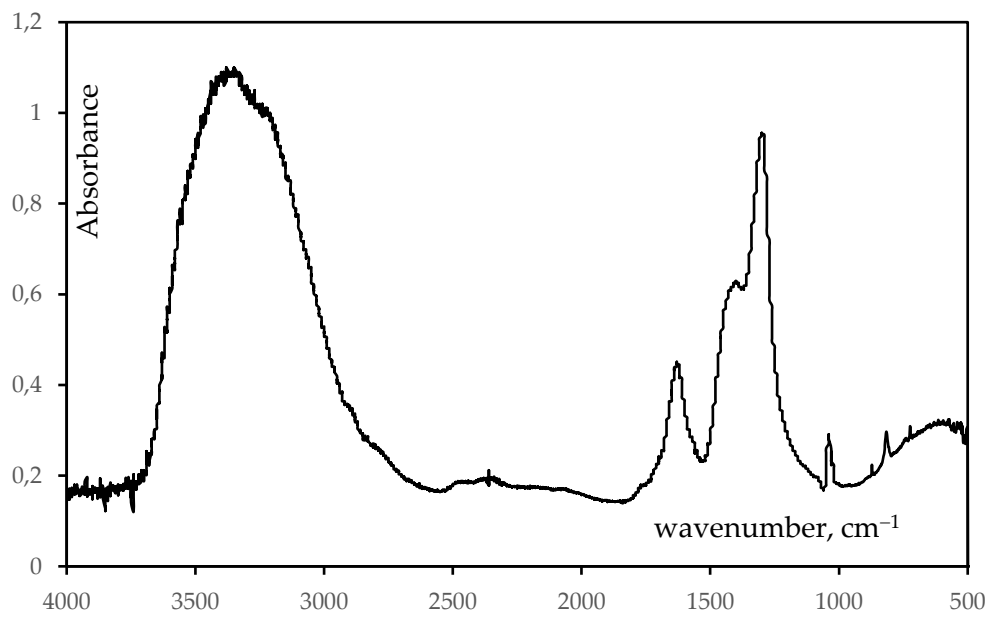
**Figure S4.** Mass spectrum ESIMS QTOF obtained by LC-MS analysis in ESI positive mode of a solution  $1.0 \times 10^{-3}$  M of harzianic acid and  $1.0 \times 10^{-3}$  M of  $\text{Pb}(\text{ClO}_4)_2$  in MeOH/ $\text{H}_2\text{O}$  50:50 ( $w/w$ ).



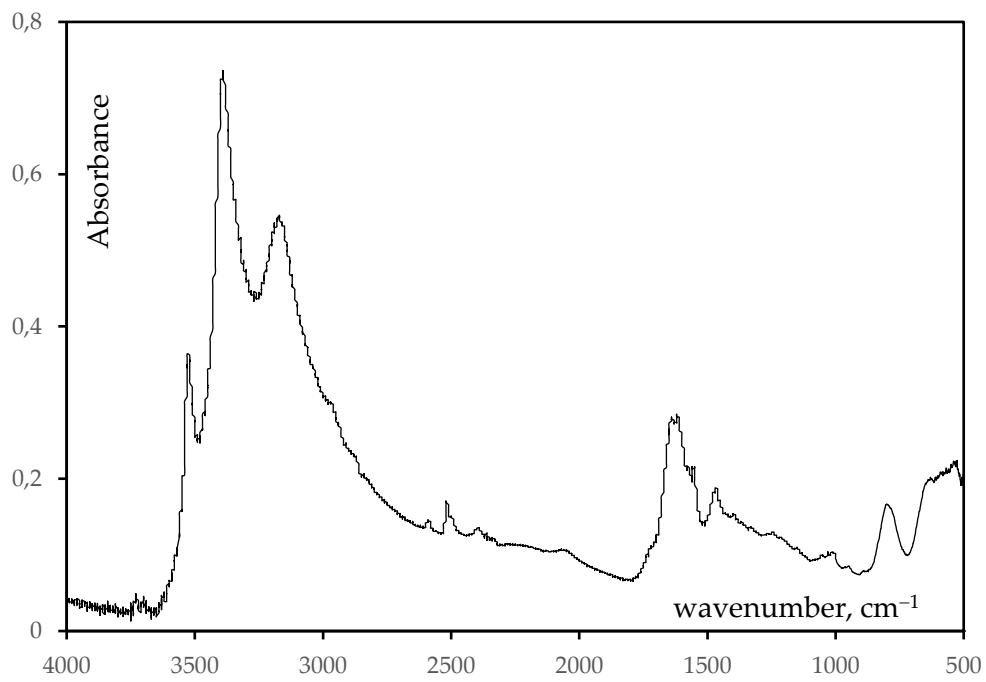
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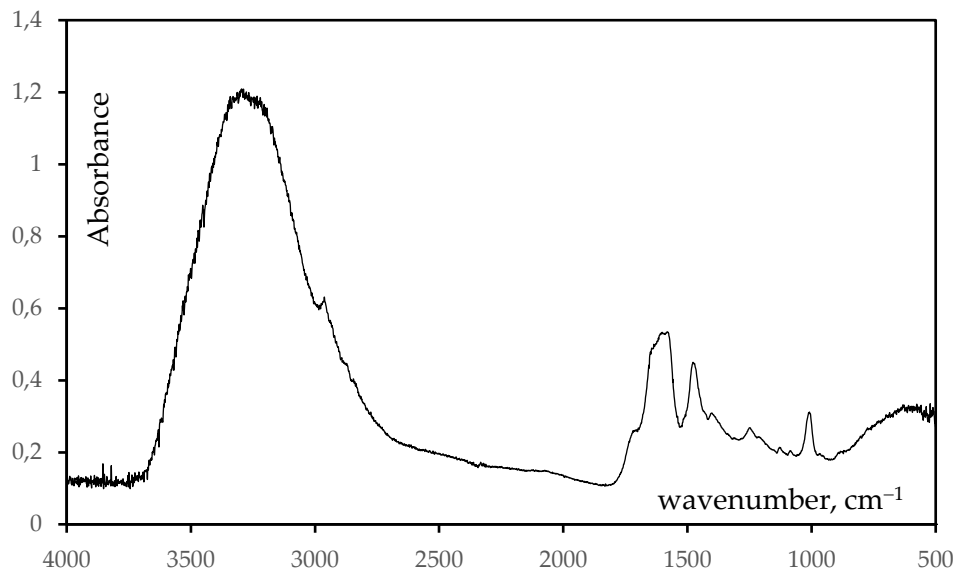
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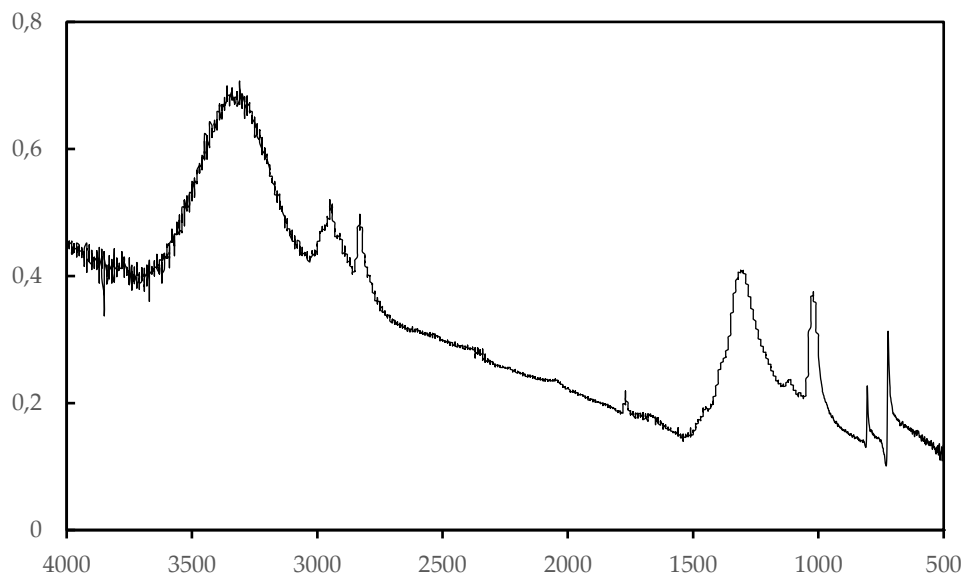
**Figure S7.** Solid-state FT-IR spectrum of Cd (II)/harzianic acid complex.



**Figure S8.** Solid-state FT-IR spectrum of Co (II)/harzianic acid complex.



**Figure S9.** Solid-state FT-IR spectrum of Ni (II)/harzianic acid complex.



**Figure S10.** FT-IR spectrum of Pb (II)/harzianic acid complex