

## Supplementary information

### **New transition metal Complexes with Indole ring pendent: Insights into the Antifungal activity and Mode of Action**

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### **Figures captions**

**Figure S1** Mass spectrum of schiff base ligand (**L**)

**Figure S2** Mass spectrum of **C1** complex

**Figure S3** Mass spectrum of **C2** complex

**Figure S4** Mass spectrum of **C3** complex

**Figure S5** Mass spectrum of **C4** complex

**Figure S6** FT-IR spectrum of **C2** complex

**Figure S7** FT-IR spectrum of **C3** complex

**Figure S8** FT-IR spectrum of **C4** complex

**Figure S9** <sup>1</sup>HNMR spectrum of Schiff base (**L**) in CDCl<sub>3</sub>

**Figure S10** <sup>1</sup>HNMR spectrum of **C4** complex in DMSO-d<sub>6</sub>

**Figure S11** <sup>13</sup>CNMR spectrum of Schiff base ligand(**L**)

**Figure S12** <sup>13</sup>CNMR spectrum of **C4** complex

**Table S1:** Effect of the test compounds (**L**, **C1-C4**) on the rate of H<sup>+</sup>-efflux by various *Candida albicans* isolates at pH 7.0: Cells were suspended in 0.1 mM CaCl<sub>2</sub> and 0.1 MKCl at 25 °C

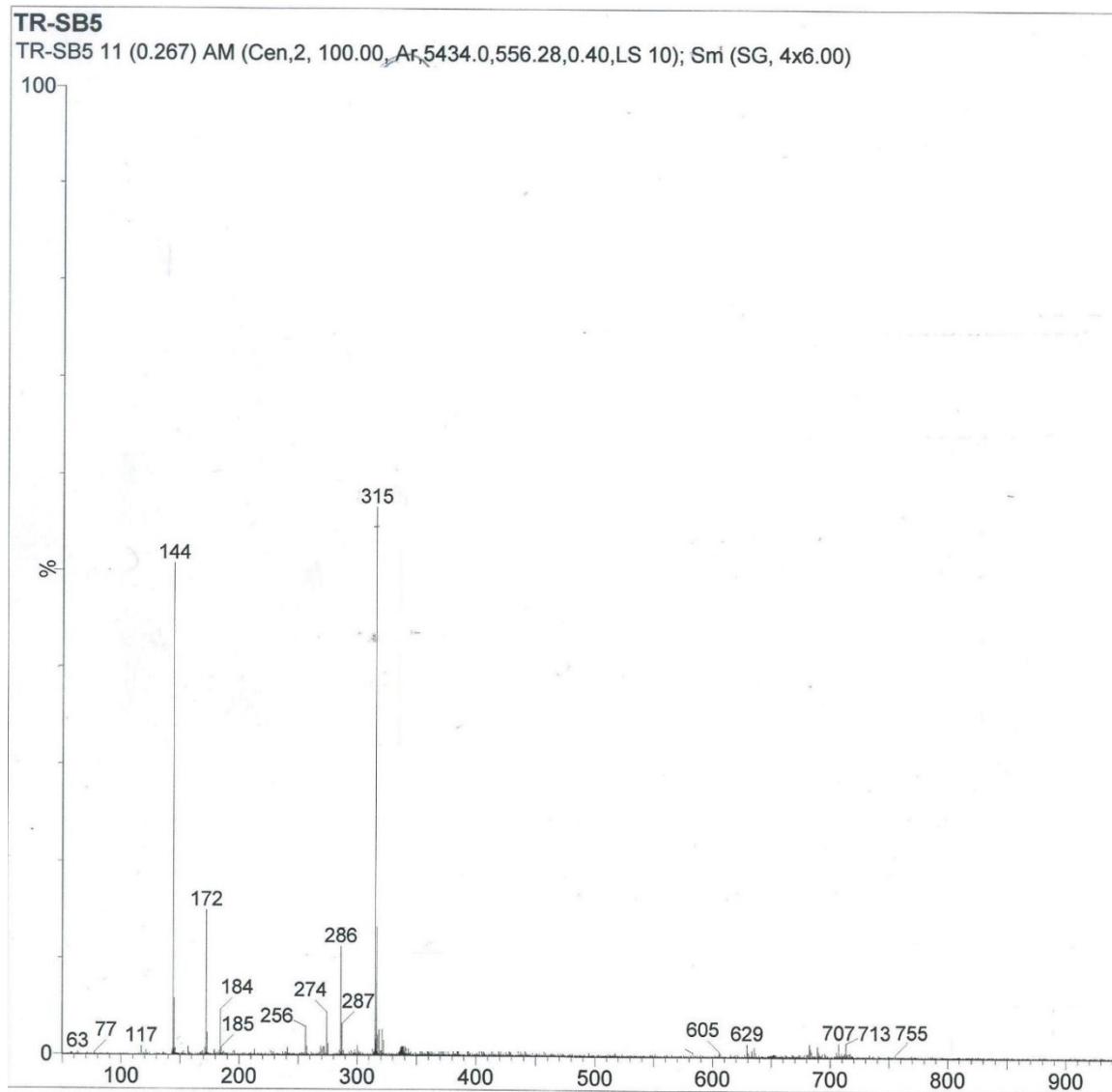
## 1. Mass spectra

The mass spectra of the Schiff base (**L**) and metal complexes (**C1-C4**) were recorded and found in good agreement with the molecular formulae and structures of these synthesized compounds. The mass spectra  $[M+H]^+$  of Schiff base ligand (**L**) showed the molecular ion peak at  $m/z$  315.0 and its corresponding metal complexes (**C1, C2, C3** and **C4**) showed molecular ion peaks at 609.5, 605.9, 605.5 and 611.4 respectively. The mass spectra of the synthesized compounds are given in **FiguresS1-S5**.

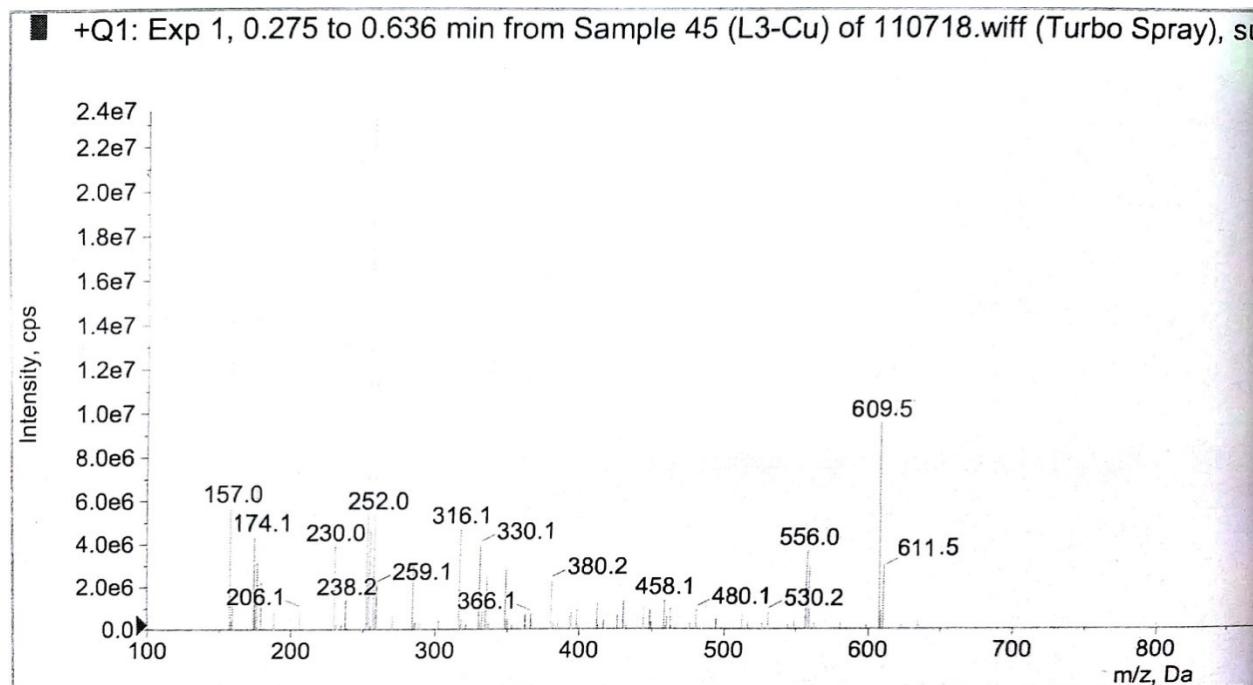
## 2. $^1\text{H}$ NMR and $^{13}\text{C}$ NMR spectra

The  $^1\text{H}$  NMR of the Schiff base (**L**) and **C4** complex was recorded in  $\text{CDCl}_3$  and  $\text{DMSO-d}_6$  respectively using tetramethylsilane (TMS) as internal standard. In Schiff base ligand (**L**) the  $\text{CH}=\text{N}$  (azomethinic) proton appeared as a singlet at 8.4 ppm and in **C4** complex the signal for the imine proton appeared at 8.53 ppm and this downfield shift with respect to the corresponding signal in the free ligand confirms the coordination of azomethine nitrogen with the Zn(II) metal ion. The Ph-OH proton of the Schiff base appeared as a singlet at 13.11 ppm. In **C4** complex the Ph-OH proton signal was found absent confirming the complexation through phenolic oxygen. The aromatic protons in Schiff base appeared as a set of multiplets in the region 6.7-8.2 ppm. The  $\text{CH}_2$  protons of the Schiff base appeared as triplets in the region 2.9-3.5 ppm. The positions of the main signals in the  $^1\text{H}$ NMR and  $^{13}\text{C}$ NMR are given in the experimental section. The attained  $^{13}\text{C}$  values of **C4** complex were compared with the corresponding ligands and were in good agreement with the proposed structure of the **C4** complex. In Schiff base the azomethine carbon atom was observed at 163.94 ppm which was shifted to 164.10 ppm in complex. The paramagnetic **C1, C2** and **C3** complexes did not show fine NMR spectra and were therefore not

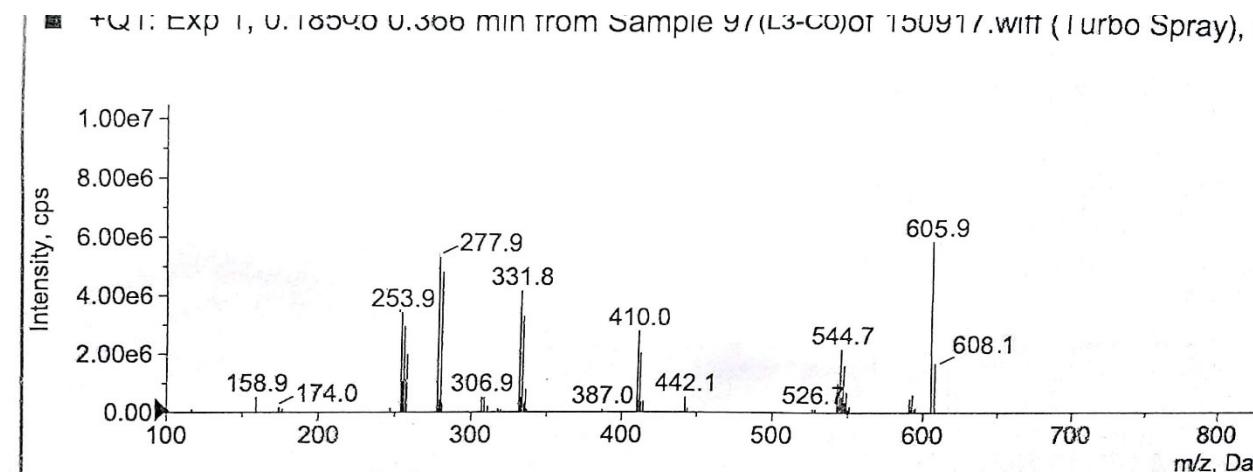
included in this study. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of Schiff base (L) and C4 complex are shown in **Figures S9-S12**.



**Figure S1** Mass spectrum of schiff base ligand (L) showing prominent parent ion peak at 315 (m/z) which corresponds to  $[\text{M}+\text{H}]^+$

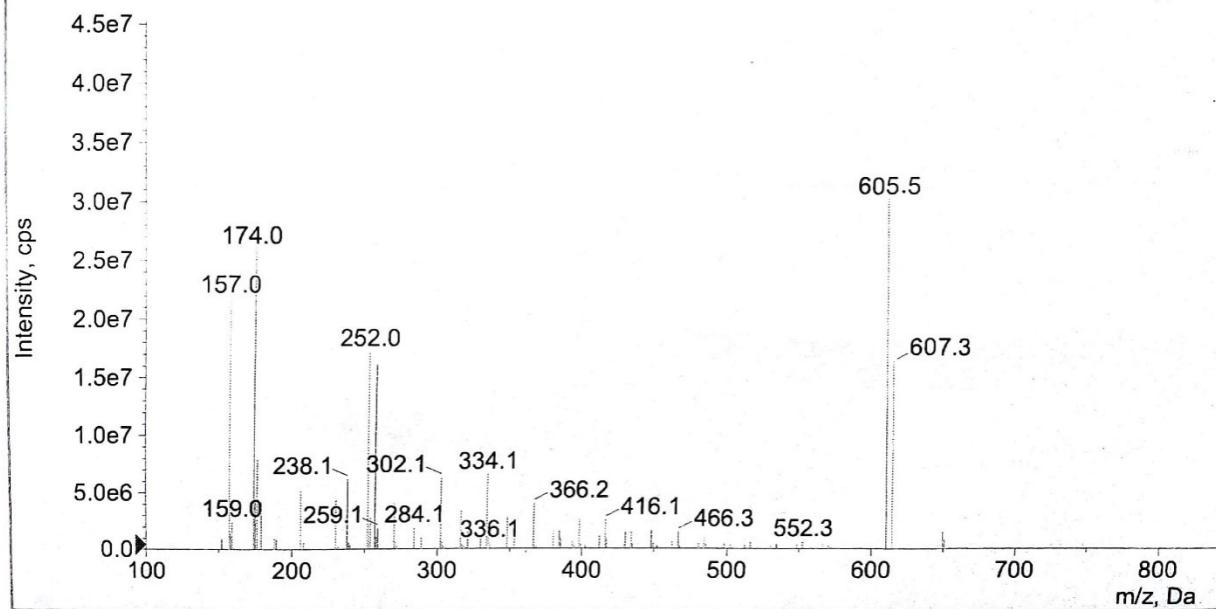


**Figure S2** Mass spectrum of C1 complex showing prominent parent ion peak at 609.5 (m/z) which corresponds to  $[M+H]^+$



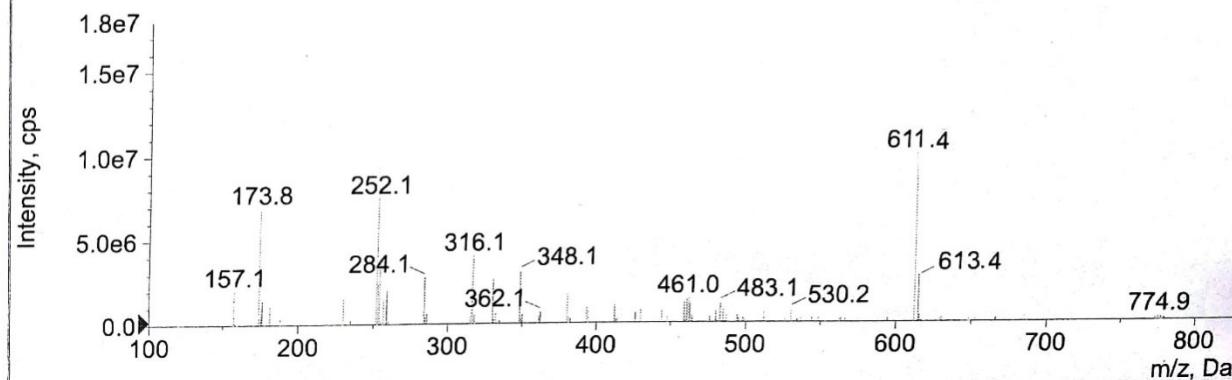
**Figure S3** Mass spectrum of C2 complex showing prominent parent ion peak at 605.9 (m/z) which corresponds to  $[M+H]^+$

■ +Q1: Exp 1, 0.366 to 0.547 min from Sample 44 (L3-NI) or 110/18.WIT (Turbo Spray),



**Figure S4** Mass spectrum of C3 complex showing prominent parent ion peak at 605.5 ( $m/z$ ) which corresponds to  $[M+H]^+$

■ +Q1: Exp 1, 0.366 to 0.637 min from Sample 34 (L3ZN) or 110/18.WIT (Turbo Spray),



**Figure S5** Mass spectrum of C4 complex showing prominent parent ion peak at 611.4 ( $m/z$ ) which corresponds to  $[M+H]^+$

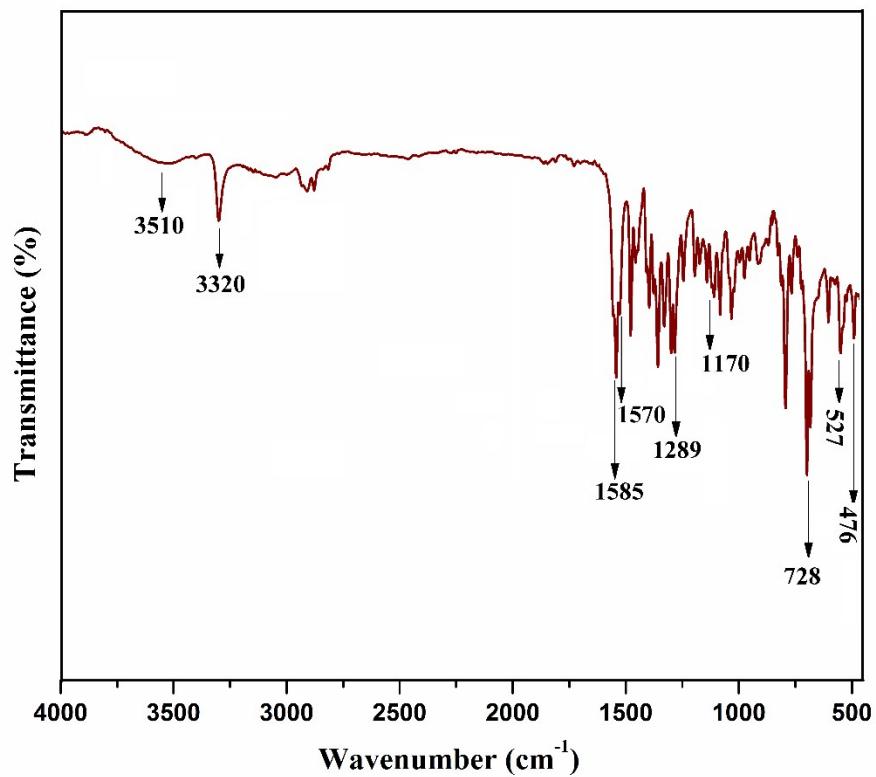


Figure S6FT-IR spectrum of C2 complex

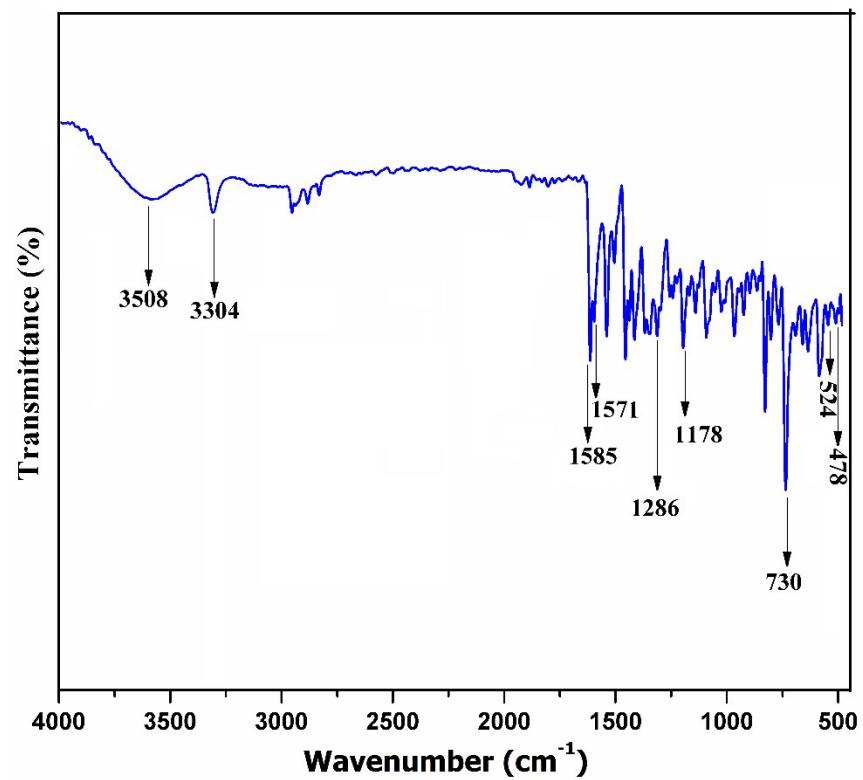
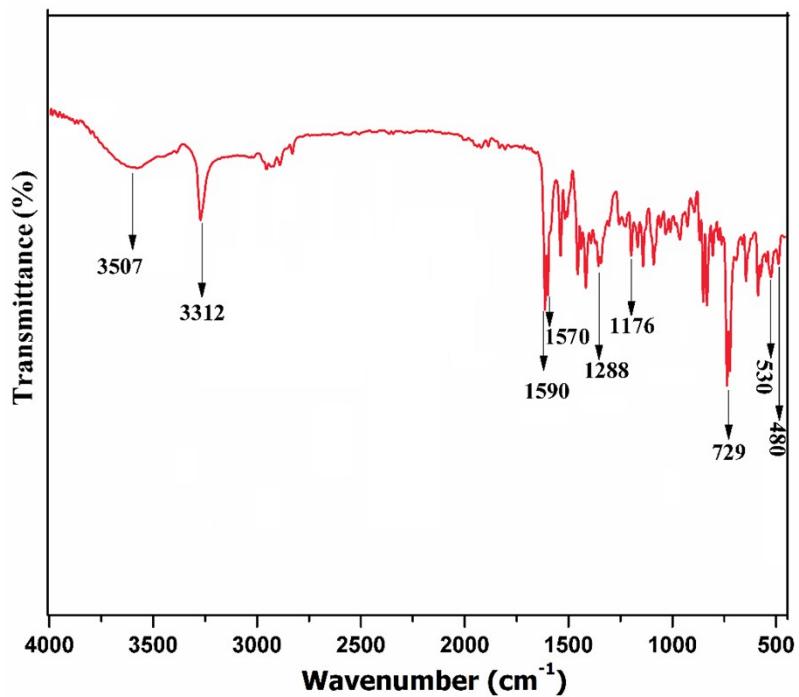
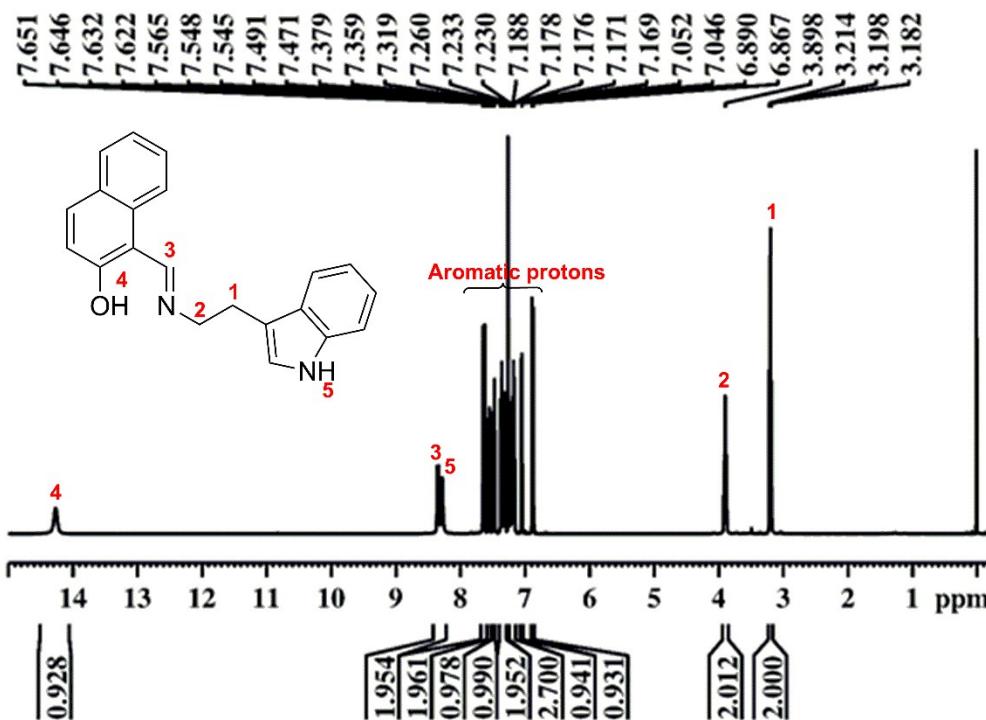


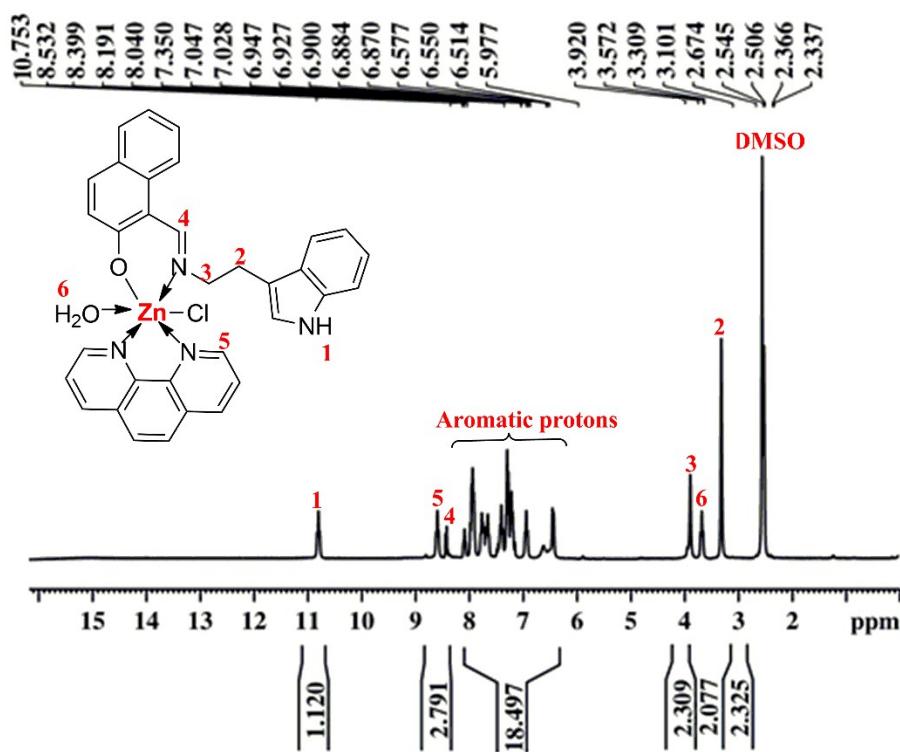
Figure S7FT-IR spectrum of C3 complex



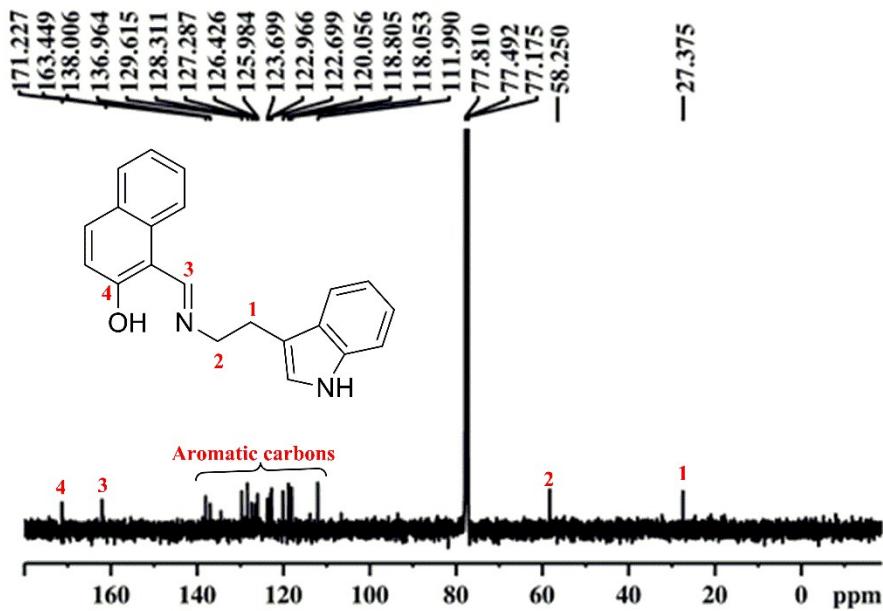
### Figure S8FT-IR spectrum of C4 complex



**Figure S9**<sup>1</sup>HNMR spectrum of Schiff base (L) in CDCl<sub>3</sub>



**Figure S10** $^1\text{H}$ NMR spectrum of **C4** complex in  $\text{DMSO-d}_6$



**Figure S11** $^{13}\text{C}$ NMR spectrum of Schiff base ligand (**L**)

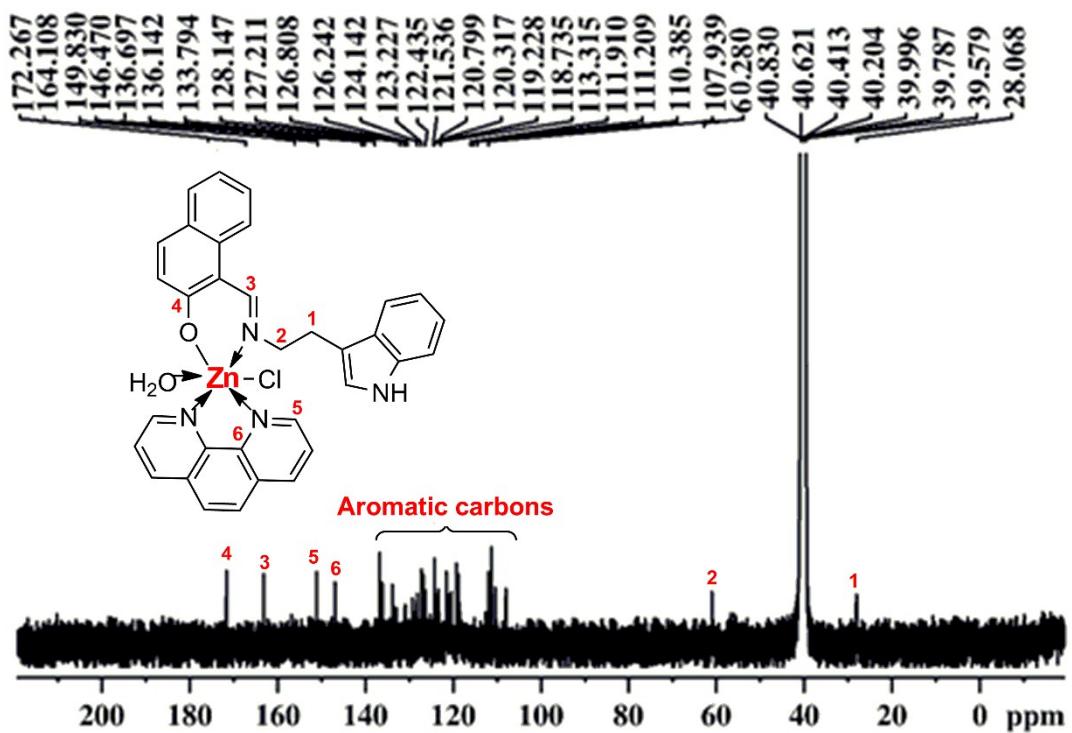


Figure S12  $^{13}\text{C}$ NMR spectra of C4 complex

**Table S1** Effect of the test compounds (L, C1-C4) on the rate of H<sup>+</sup>-efflux by various *Candida albicans* isolates at pH 7.0: Cells were suspended in 0.1 mM CaCl<sub>2</sub> and 0.1 MKCl at 25 °C

| Test compounds       | Range of relative H <sup>+</sup> -efflux rate (×10 <sup>-11</sup> mol/min/mg cells) |               |               |               |               |               |               |               |                       |               |               |
|----------------------|---|---------------|---------------|---------------|---------------|---------------|---------------|---------------|-----------------------|---------------|---------------|
|                      | FLC Susceptible strains   |               |               |               |               |               |               |               | FLC Resistant strains |               |               |
|                      | SC5314  | 4175          | 4179          | 4180          | 4251          | 4554          | 4563          | 4576          | 4085                  | 4122          | 4135          |
| <b>Control</b>       | 4.131   | 5.642         | 5.861         | 6.124         | 5.113         | 5.772         | 6.193         | 5.911         | 9.043                 | 8.442         | 8.341         |
| <b>Glucose(5 mM)</b> | 11.34   | 11.89         | 12.71         | 12.48         | 11.22         | 12.32         | 13.57         | 12.61         | 22.99                 | 21.37         | 21.54         |
| <b>L</b>             | 3.038<br>(27)   | 3.923<br>(31) | 4.577<br>(22) | 4.673<br>(24) | 4.003<br>(19) | 4.237<br>(27) | 4.787<br>(23) | 4.451<br>(25) | 5.362<br>(41)         | 5.259<br>(38) | 5.246<br>(37) |
| <b>L+Glucose</b>     | 9.331<br>(18)   | 9.429<br>(21) | 10.68<br>(16) | 9.772<br>(12) | 10.01<br>(11) | 10.01<br>(19) | 11.61<br>(15) | 10.61<br>(16) | 18.23<br>(21)         | 17.51<br>(18) | 6.181<br>(26) |
| <b>C1</b>            | 3.033<br>(27)   | 3.886<br>(31) | 4.588<br>(22) | 4.673<br>(24) | 4.029<br>(19) | 4.219<br>(27) | 4.156<br>(23) | 4.451<br>(25) | 6.520<br>(28)         | 6.441<br>(24) | 6.781<br>(19) |
| <b>C1+Glucose</b>    | 9.296<br>(18)   | 9.429<br>(21) | 10.68<br>(16) | 9.834<br>(12) | 10.02<br>(11) | 9.992<br>(19) | 11.57<br>(15) | 10.58<br>(16) | 18.23<br>(21)         | 19.63<br>(19) | 6.923<br>(17) |
| <b>C2</b>            | 4.689<br>(59)   | 2.098<br>(63) | 2.778<br>(53) | 2,639<br>(57) | 2.623<br>(49) | 2.869<br>(51) | 2.768<br>(56) | 2.843<br>(52) | 2.830<br>(69)         | 2.820<br>(67) | 3.028<br>(64) |
| <b>C2+Glucose</b>    | 7.563<br>(44)   | 6.325<br>(47) | 5.783<br>(55) | 6.402<br>(49) | 6.698<br>(41) | 4.078<br>(67) | 6.391<br>(53) | 7.226<br>(43) | 8.989<br>(61)         | 6.582<br>(69) | 2.94<br>(65)  |
| <b>C3</b>            | 0.983<br>(67)   | 1.602<br>(72) | 2.174<br>(63) | 2,652<br>(57) | 1.416<br>(53) | 2.372<br>(59) | 2.558<br>(59) | 2.288<br>(62) | 1.709<br>(81)         | 1.849<br>(78) | 1.843<br>(78) |
| <b>C3+Glucose</b>    | 5.635<br>(51)   | 5.125<br>(57) | 6.266<br>(51) | 3.456<br>(63) | 4.645<br>(59) | 6.542<br>(47) | 6.120<br>(55) | 4.843<br>(62) | 7.380<br>(68)         | 7.971<br>(63) | 2.761<br>(67) |
| <b>C4</b>            | 3.161<br>(24)   | 2.882<br>(49) | 4.178<br>(29) | 4,862<br>(21) | 4.407<br>(24) | 3.873<br>(33) | 4.279<br>(31) | 4.498<br>(24) | 6.339<br>(30)         | 6.171<br>(27) | 5.747<br>(31) |
| <b>C4+Glucose</b>    | 9.632<br>(15)   | 7.027<br>(41) | 10.11<br>(21) | 10.75<br>(14) | 9.391<br>(17) | 9.400<br>(24) | 10.62<br>(22) | 10.78<br>(15) | 17.95<br>(22)         | 17.83<br>(17) | 6.056<br>(27) |
| <b>Fluconazole</b>   | 3.571<br>(14)   | 4.585<br>(19) | 5.233<br>(11) | 5.469<br>(11) | 4.566<br>(13) | 4.571<br>(21) | 5.456<br>(12) | 5.385<br>(09) | 8.130<br>(10)         | 7.758<br>(08) | 7.582<br>(10) |

Values in parentheses give the %-age inhibition of H<sup>+</sup>-efflux w.r.t. control