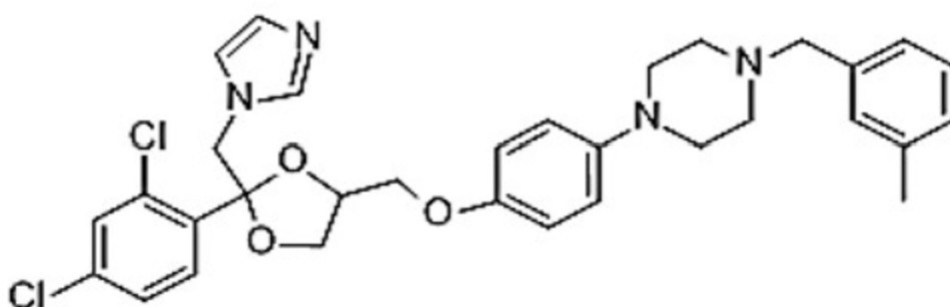


**Title** - Synthesis, characterization, and biological activity of novelazole piperazine congeners

**SUPPLEMENTARY MATERIAL**

For all four synthesized molecules (KTZ-1, KTZ-2, ITZ-1, and ITZ-2), a separate file is attached containing their respective:

1. <sup>1</sup>HNMR,
2. FTIR,
3. LCMS graphs and
4. ZOI (Zone of Inhibition) plate images against all three pathogens and control.



Solvent: dmsc  
SA-Varian 400MHz NMR  
Date: Mar 19 2022

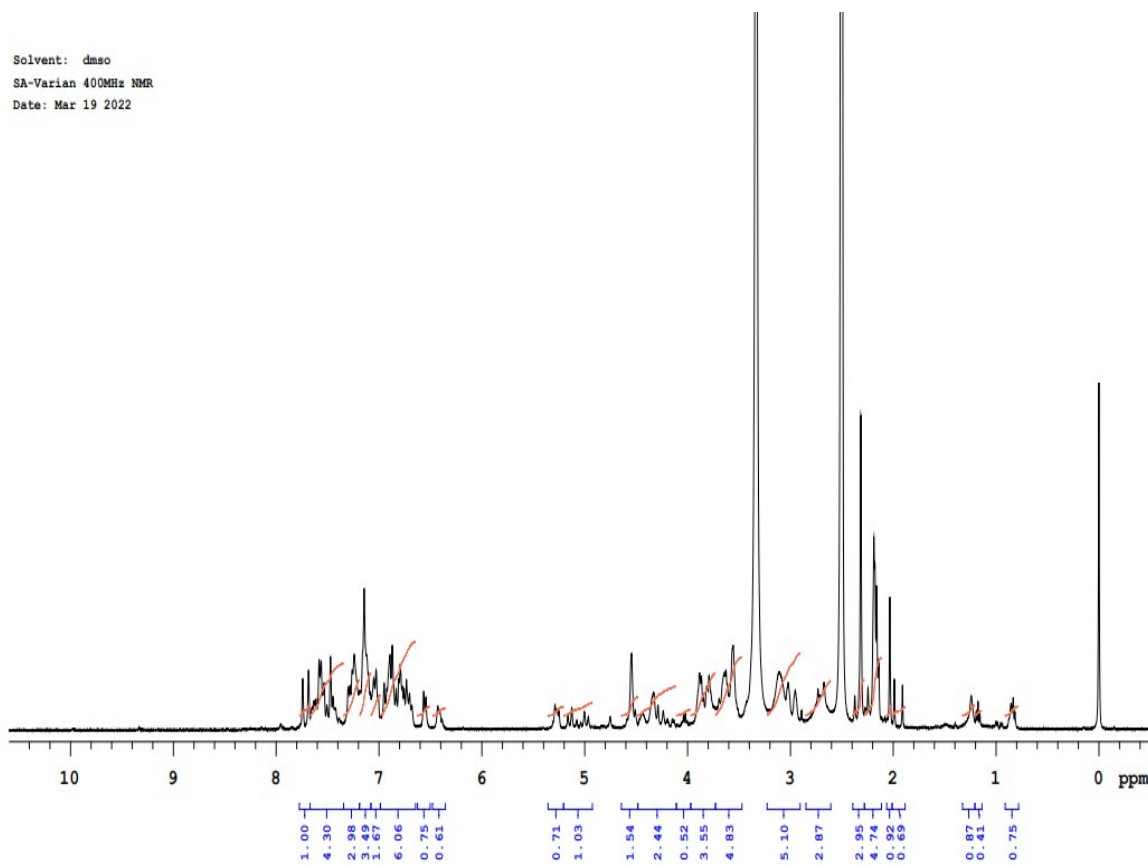


Figure 1. <sup>1</sup>H NMR data of KTZ-1 in DMSO

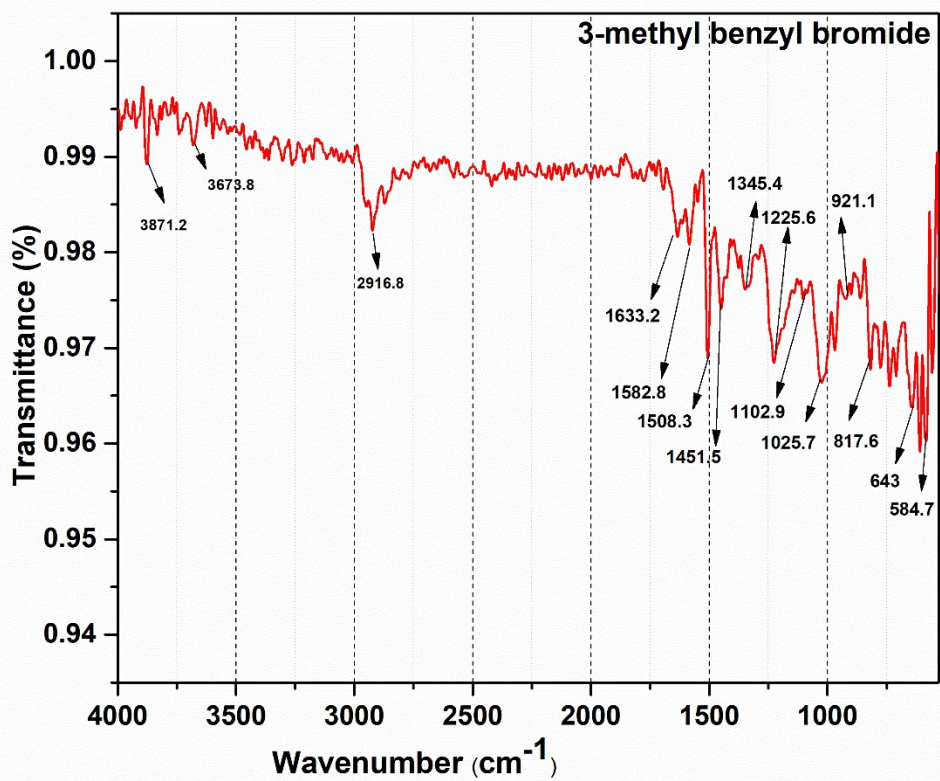
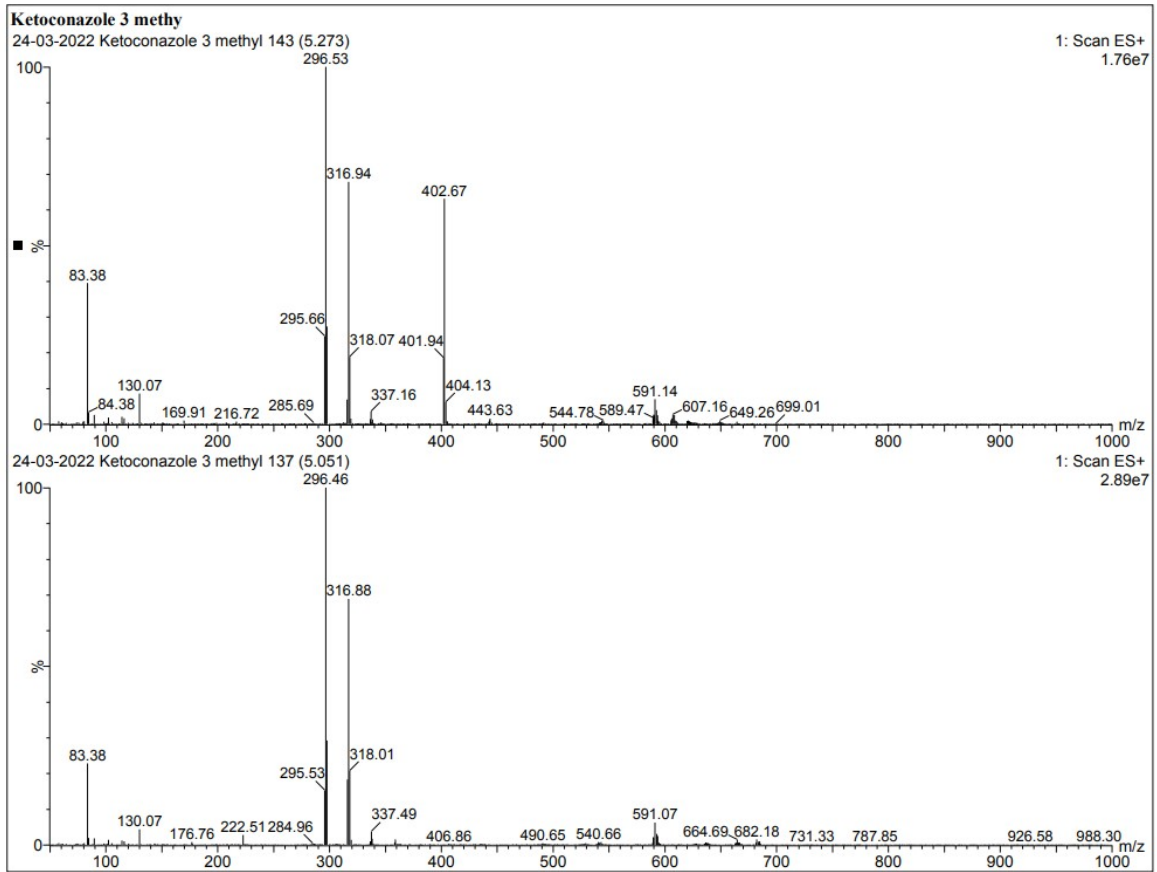
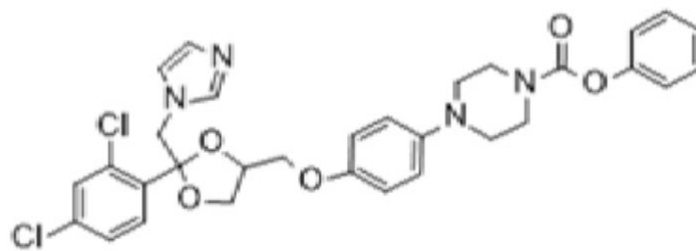


Figure 2. FTIR data of KTZ-1



**Figure 3. LCMS data of KTZ-1**



Solvent: dmsc  
SA-Varian 400MHz NMR  
Date: Mar 19 2022

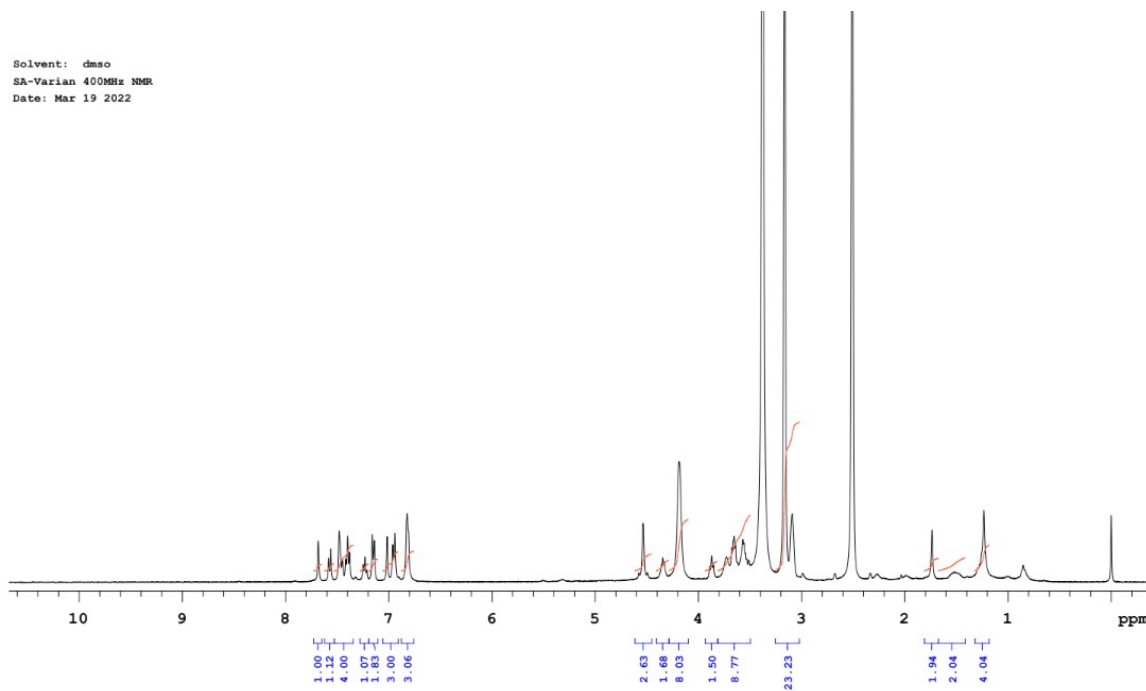


Figure 4. <sup>1</sup>H NMR data of KTZ-2 in DMSO

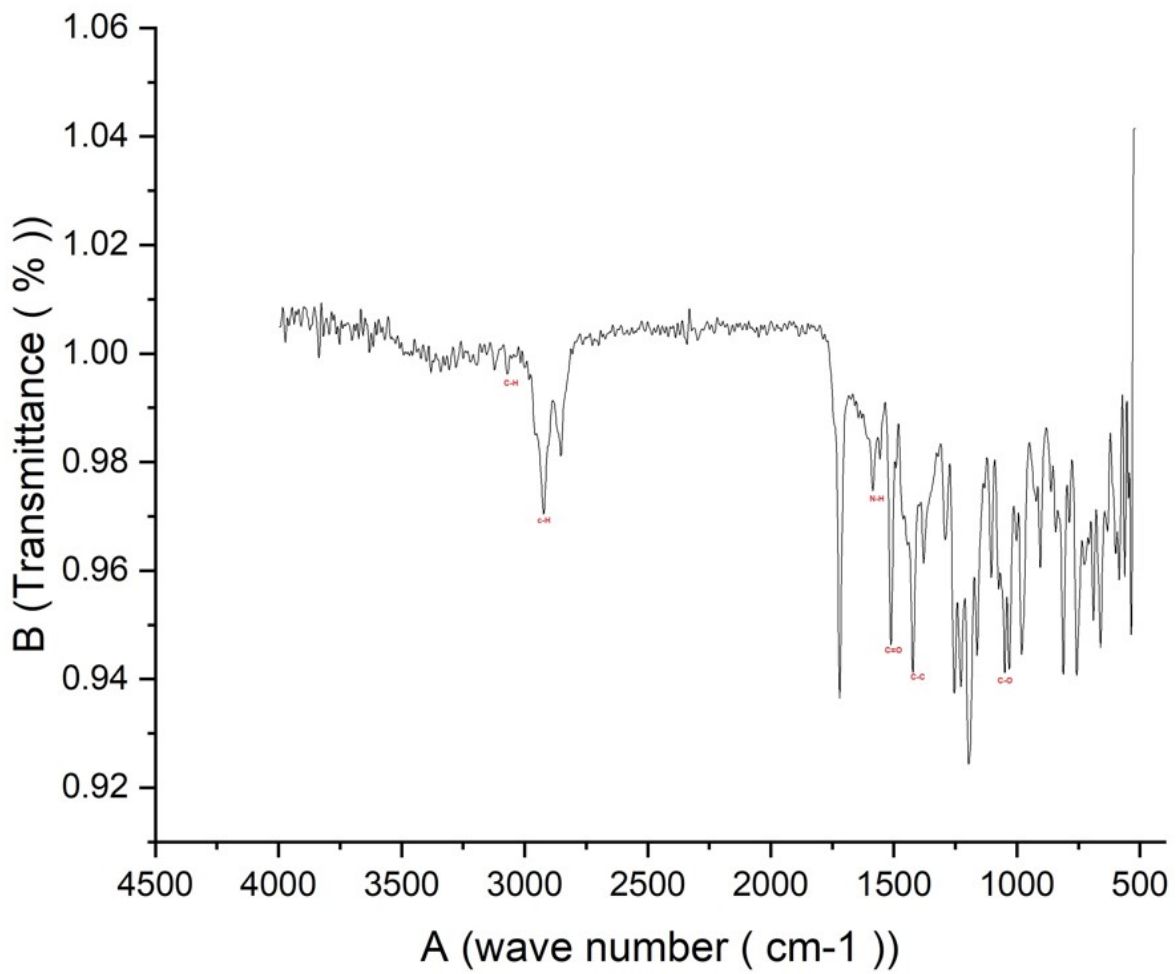
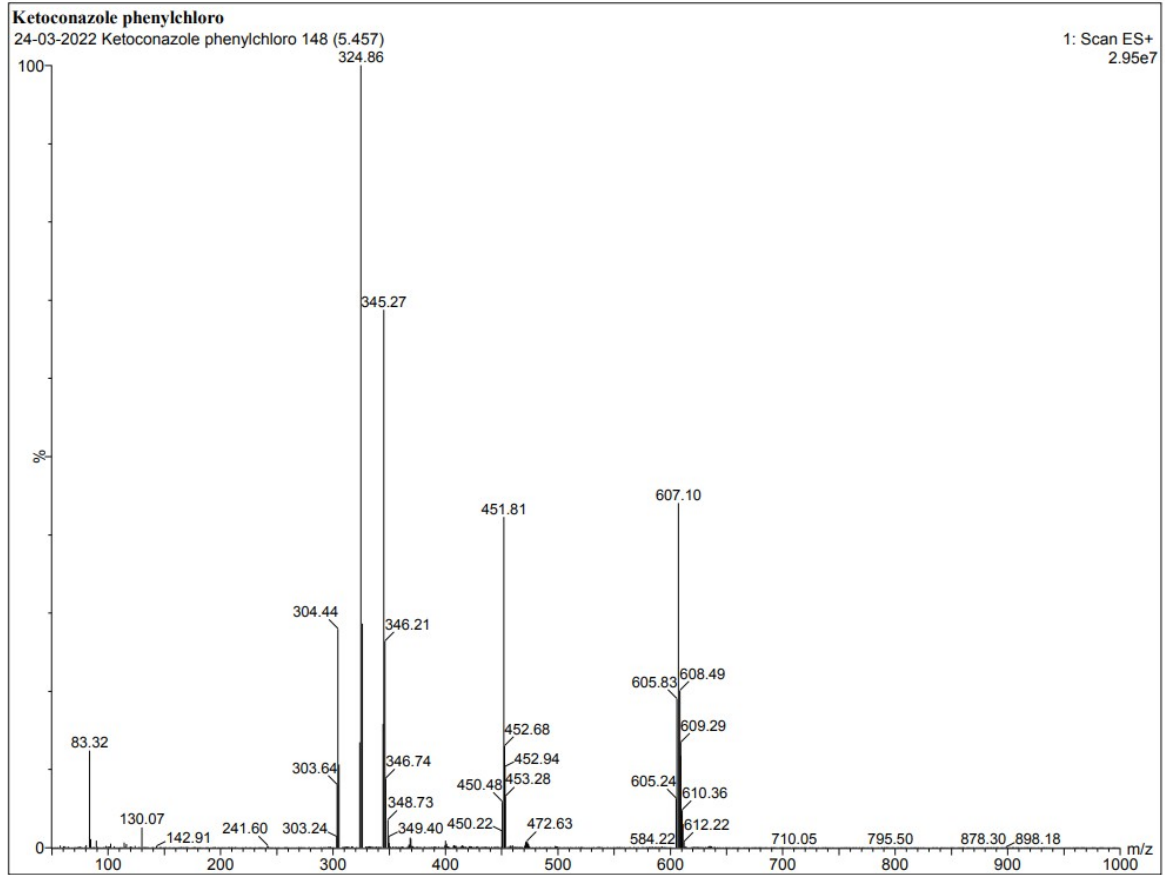
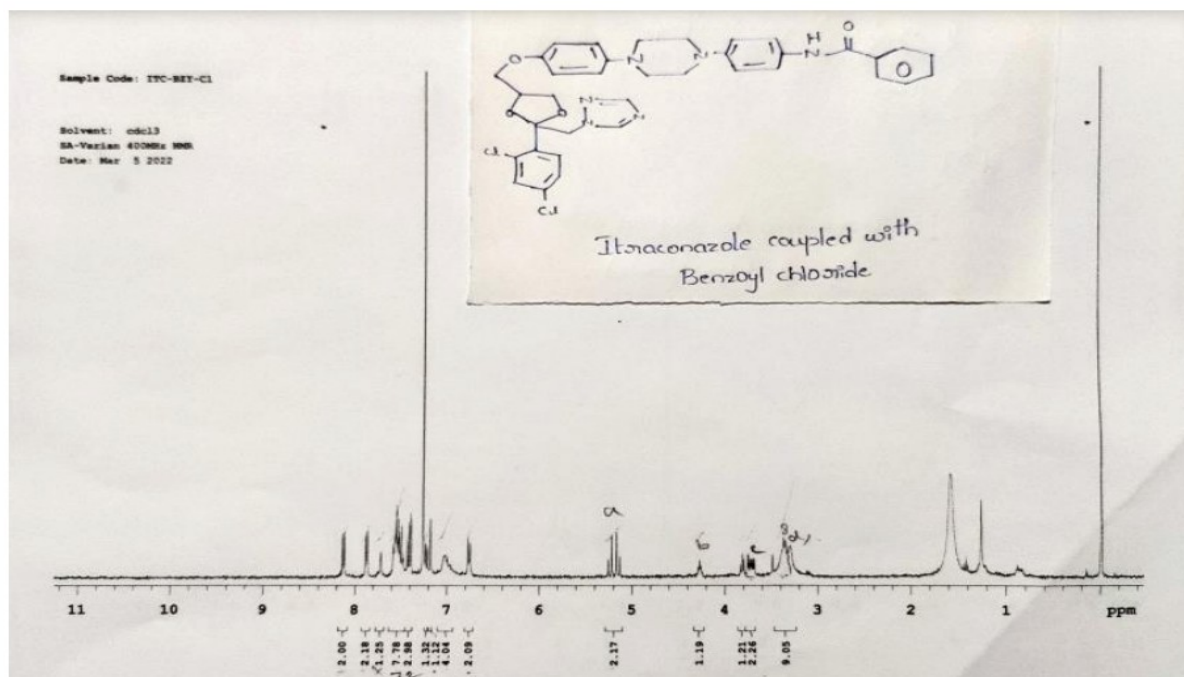


Figure 5. FTIR data of KTZ-2



**Figure 6. LCMS data of KTZ-2**



$^1\text{H NMR}$ :  $\delta$  – 3.6 (2H,  $J$  = 5, piperazine ring),  $\delta$  – 3.7 (2H,  $J$  = 3, 1,3 dioxalan),  $\delta$  – 3.8 (s  $J$  = 6, R-OCH<sub>3</sub>),  $\delta$  – 4.2 (s, Oxygenated bridge),  $\delta$  – 5.2 (s, amide linkage), 6.8 to 8.2 ( $J$  – 2 to 9 aromatic rings),  $\delta$  – 8.1 (s, 1,2,4 triazole),  $\delta$ -7.8 ( $J$  = 7, benzene attached with chlorine),  $\delta$ -6.8( $J$  = 9, Benzene attached to Nitrogen)

**Figure 7.  $^1\text{NMR}$  data of ITZ-1 in  $\text{CDCl}_3$**



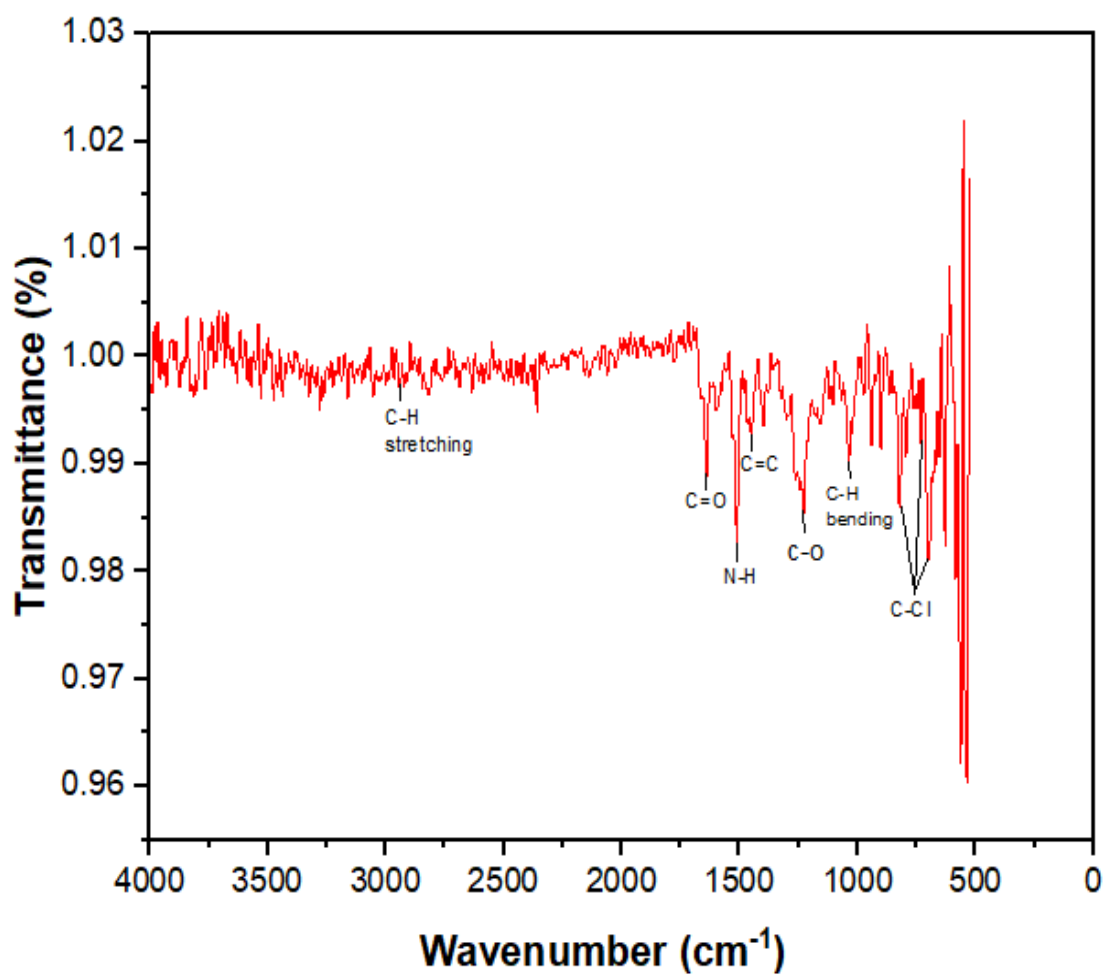


Figure 8. FTIR data of ITZ-1

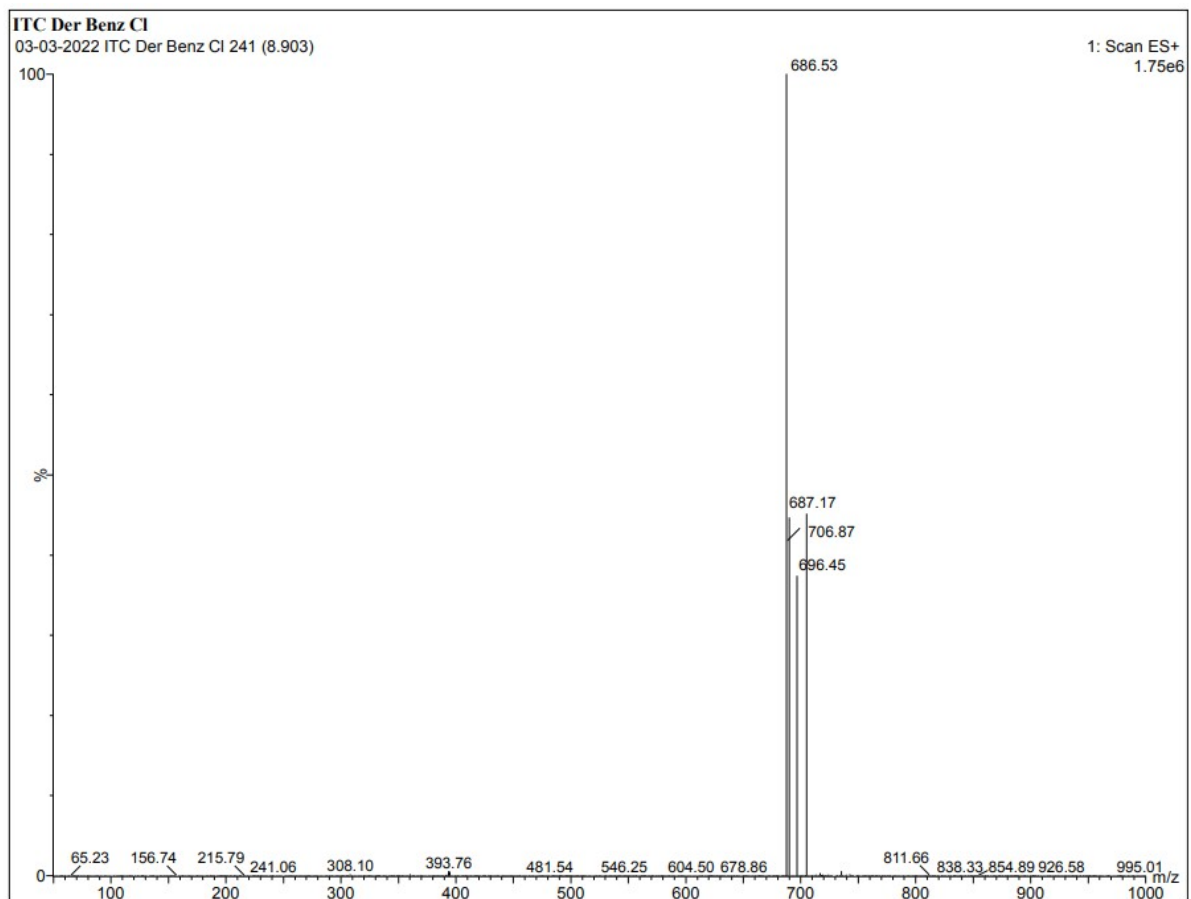
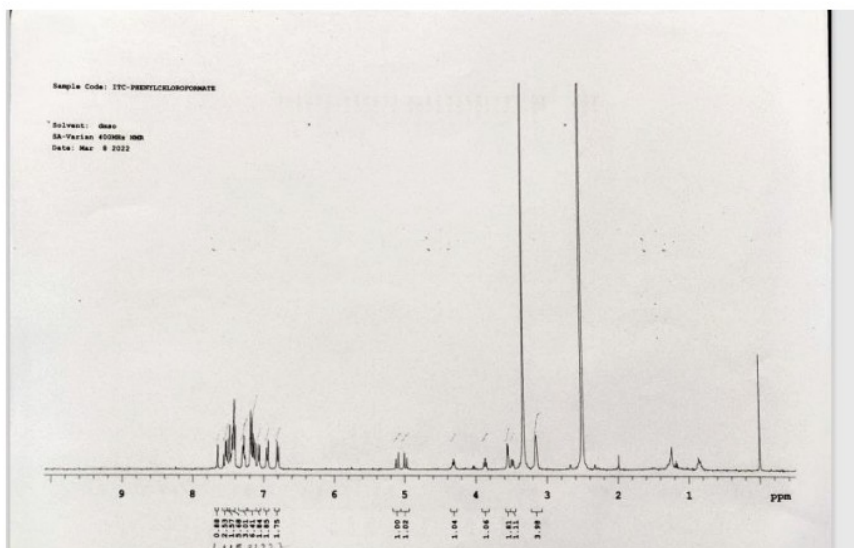


Figure 9. LCMS data of ITZ-1



$^1\text{H}$  NMR:  $\delta$  – 3.6 (2H,  $J$  = 5, piperazine ring),  $\delta$  – 3.7 (2H,  $J$  = 3, 1,3 dioxalan),  $\delta$  – 3.8 (s  $J$  = 6, R- $\text{OCH}_3$ ),  $\delta$  – 4.2 (s, Oxygenated bridge),  $\delta$  – 5.2 (s, ester-amide linkage), 6.8 to 8.2 ( $J$  – 2 to 9 aromatic rings),  $\delta$  – 8.1 (s, 1,2,4 triazole),  $\delta$ -7.8 ( $J$  = 7, benzene attached with chlorine),  $\delta$ -6.8( $J$  = 9, Benzene attached to Nitrogen)

**Figure 10.  $^1\text{H}$ NMR data of ITZ-2 in DMSO**

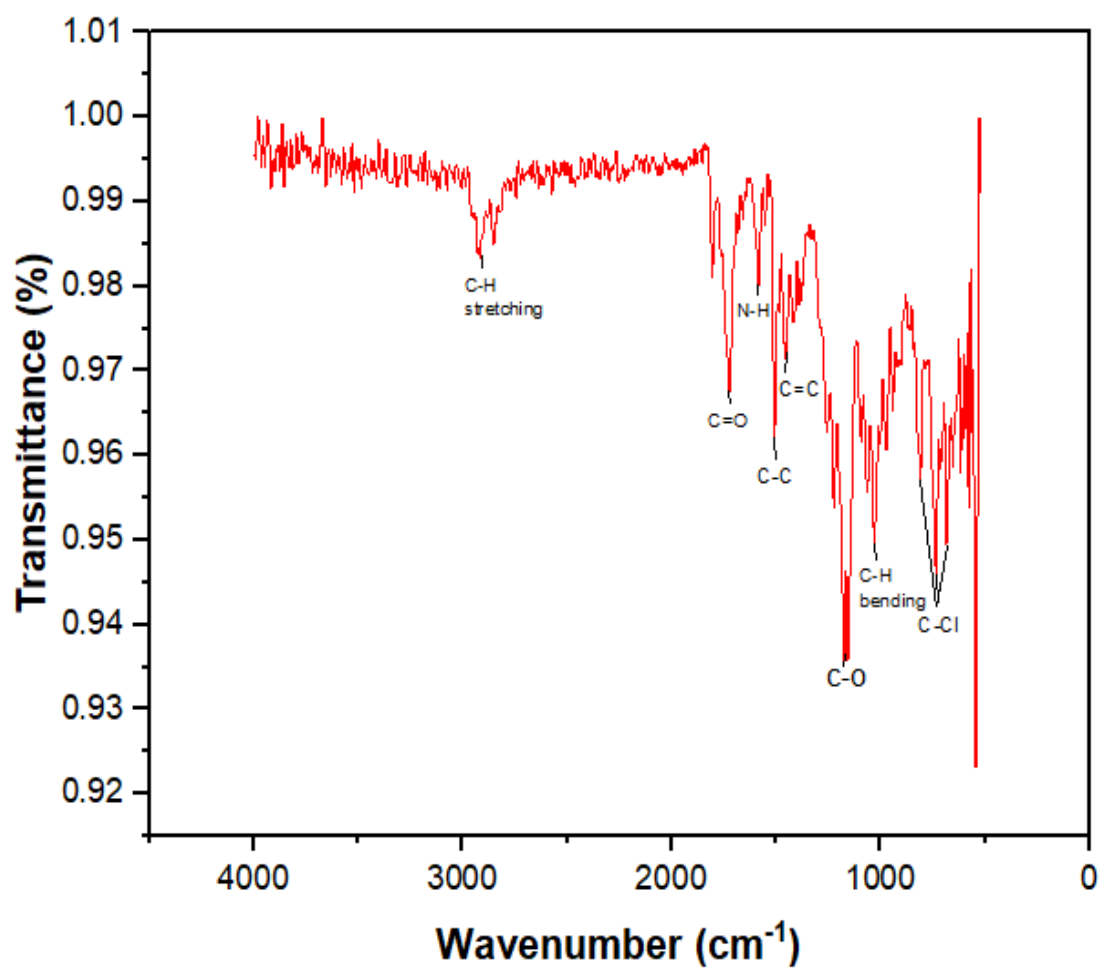
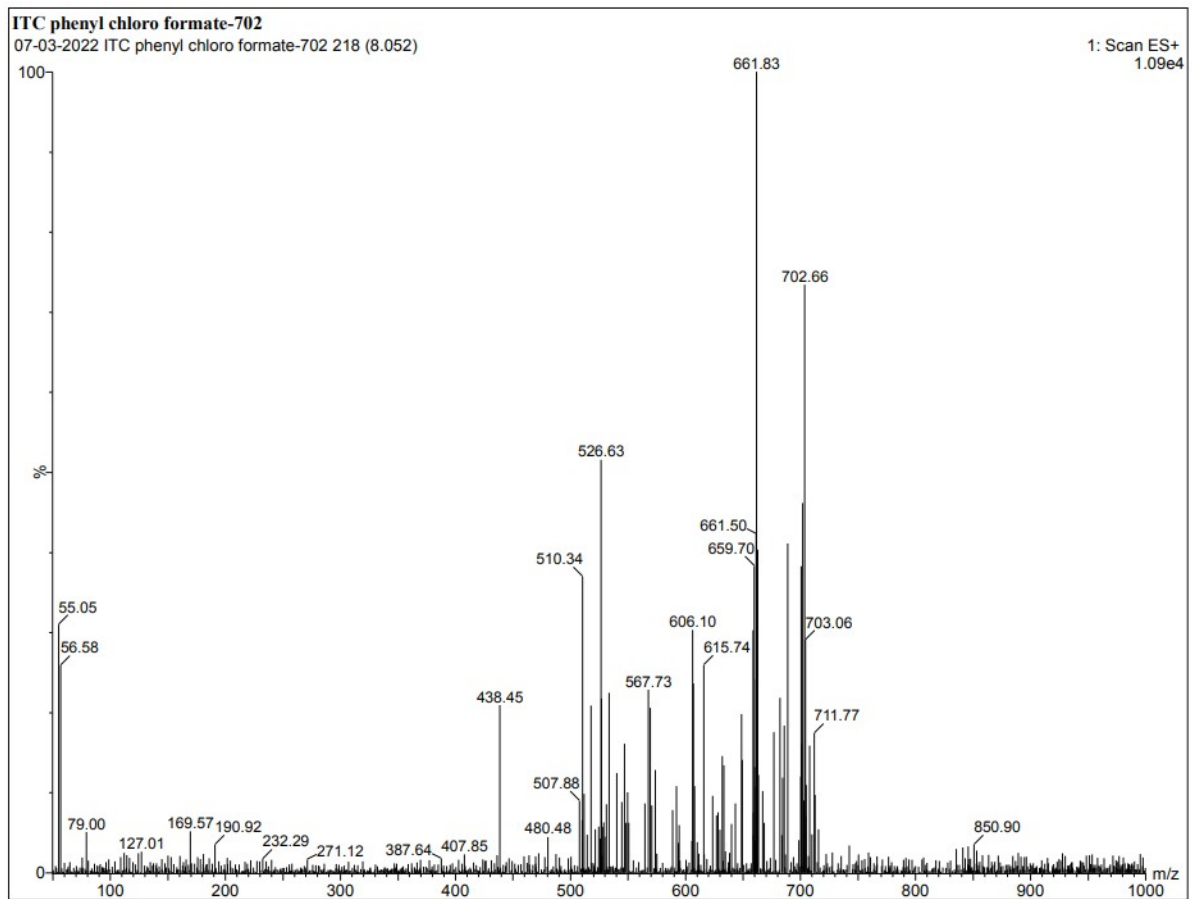
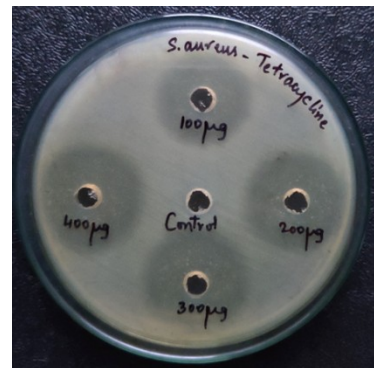


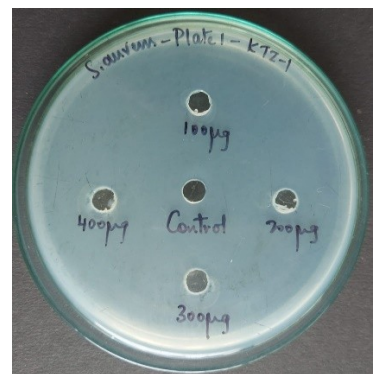
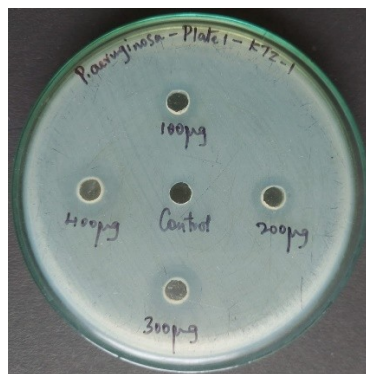
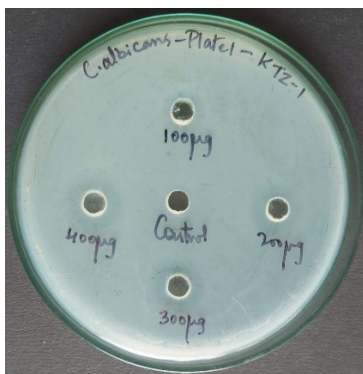
Figure 11. FTIR data of ITZ-2



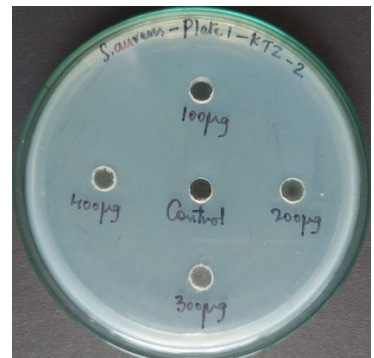
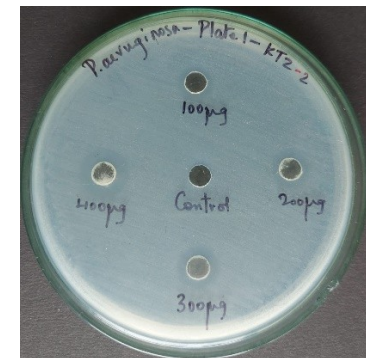
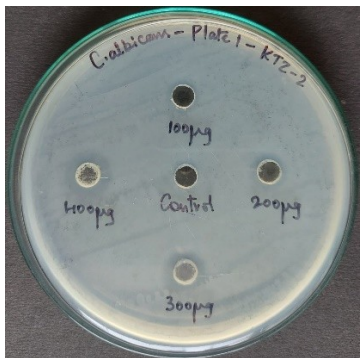
**Figure 12. LCMS data of ITZ-2**



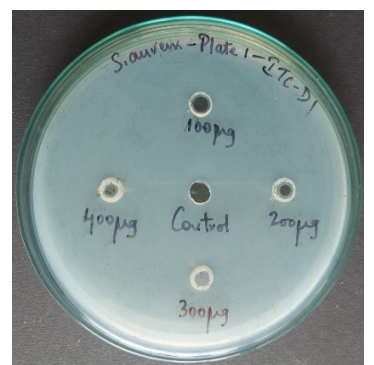
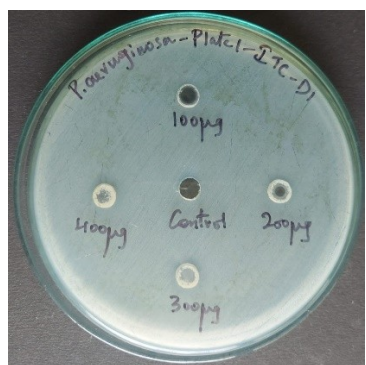
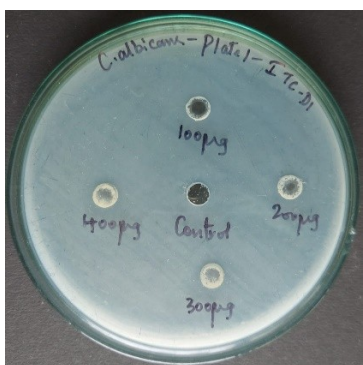
13a. Tetracycline (control group)



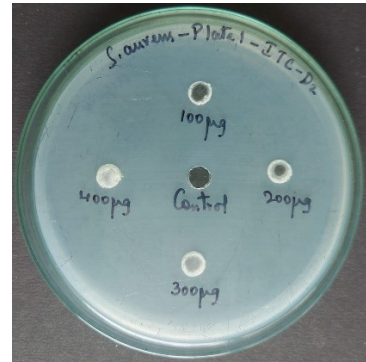
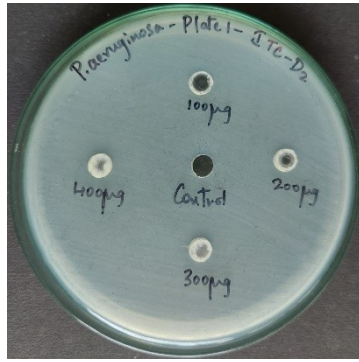
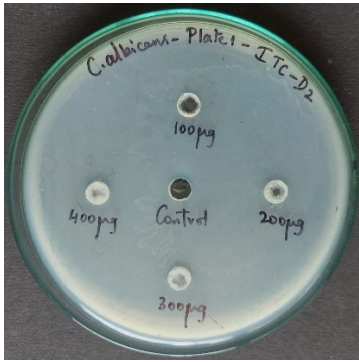
13b. KTZ-1



13c. KTZ-2



**13d.ITZ-1**



**13e.ITZ-2**

**Figure 13. MIC plate images of 13a.Tetracycline (control group), 13b.KTZ-1, 13c.KTZ-2, 13d.ITZ-1 and 13e. ITZ-2 against pathogens**