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# Synthesis, Characterisation and Evaluation of Novel Antibacterial Agents

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## Abstract

Among the transition metal complexes, ruthenium-based complexes have been widely studied and some have displayed significant antibacterial activity. This can be due to their ability to; strongly bind nucleic acids and proteins, ligand exchange kinetics similar to those of their platinum counterparts, the prevalence of two main oxidation states (II and III) and the iron-mimicking property when bound to biological molecules.<sup>1,2</sup> However, only very recently studies have shown significant interest in their antimicrobial properties.<sup>3,4</sup>

A series of novel octahedral Ru (II) complexes with varying auxiliary ligands, (L1) 2, 2'-bipyridine, and 1, 10-phenanthroline were synthesised bound to a series of systematically varied polypyridyl ligand (L2), of the form  $[\text{Ru}(\text{L}1)_2\text{L}2](\text{PF}_6)_2$ .<sup>5</sup>

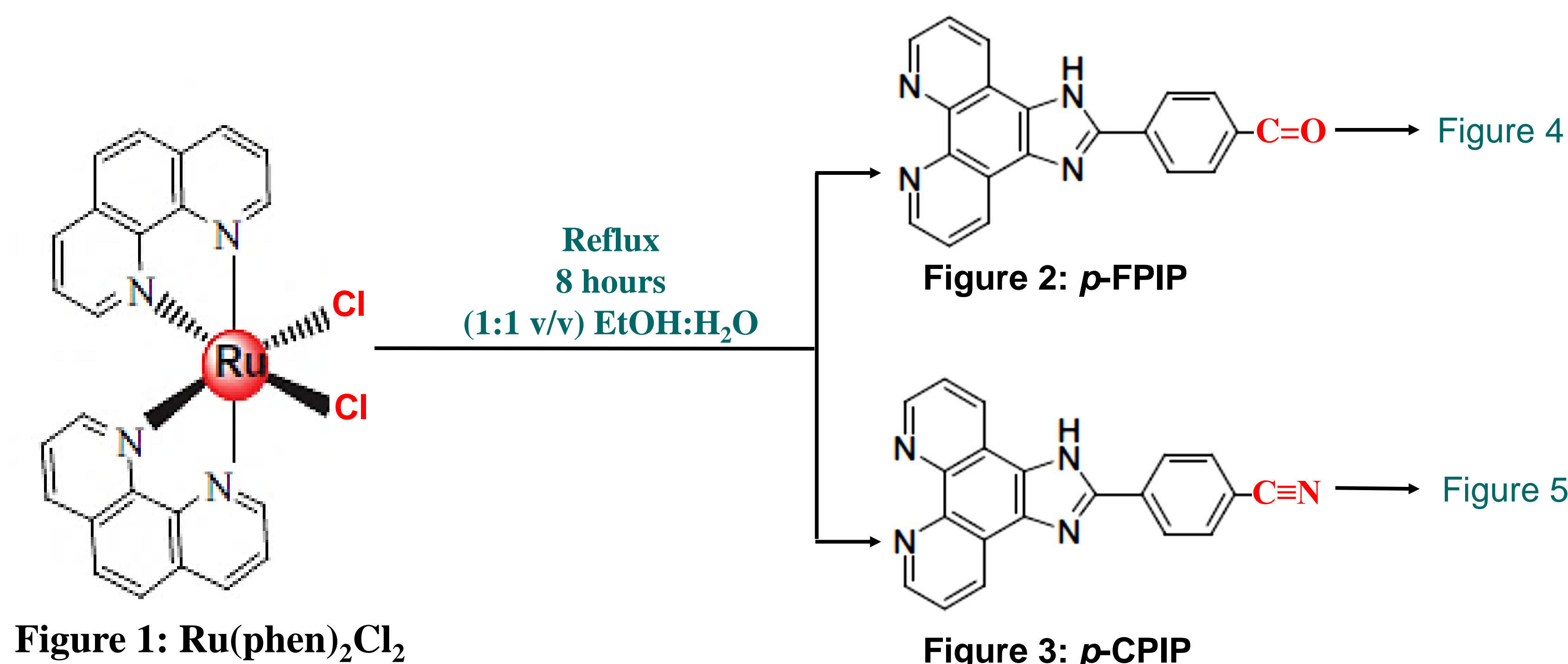


Figure 1:  $\text{Ru}(\text{phen})_2\text{Cl}_2$

Figure 3:  $p\text{-CPIP}$

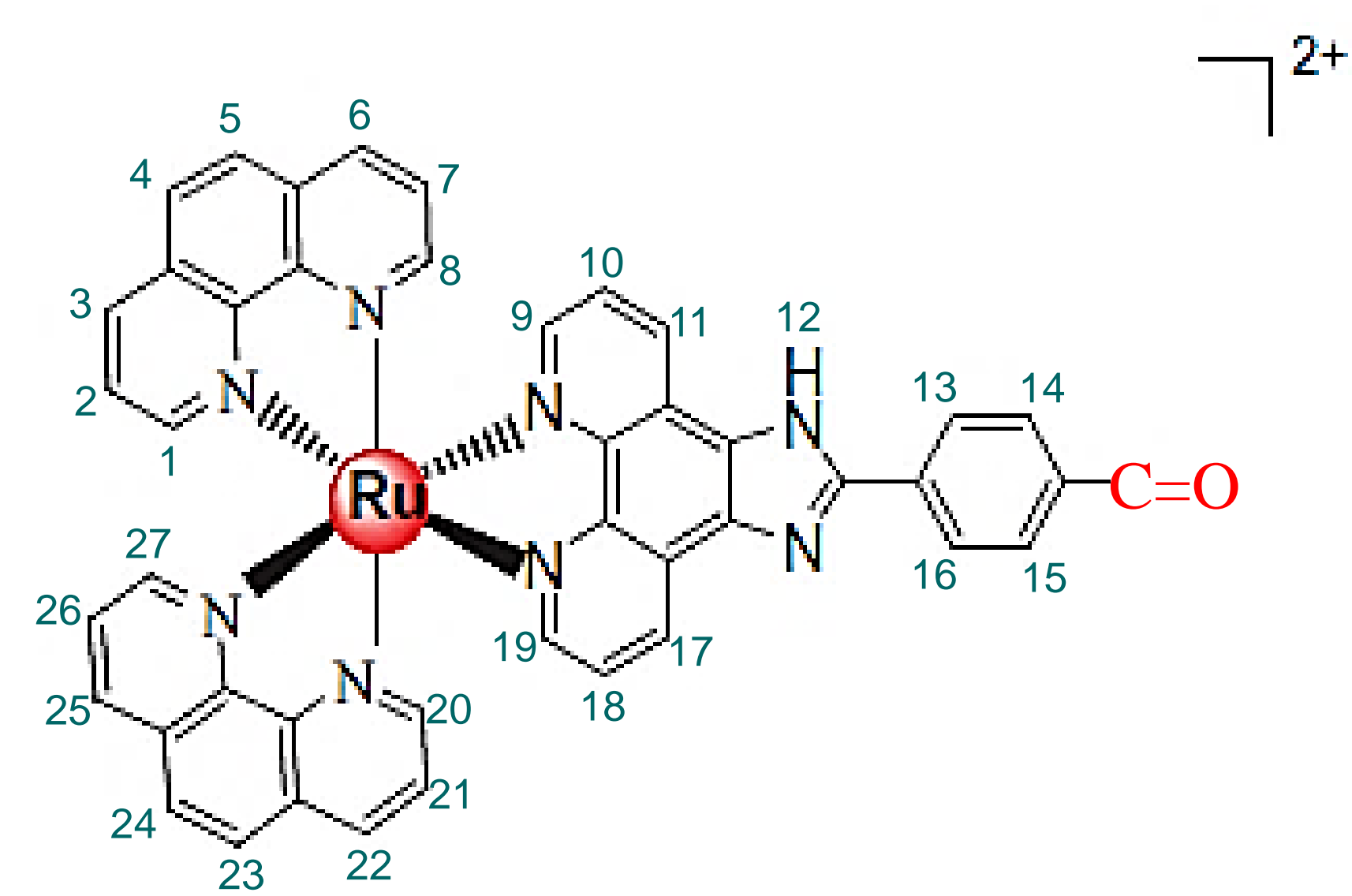


Figure 4:  $[\text{Ru}(\text{phen})_2p\text{-FPIP}]^{2+}$

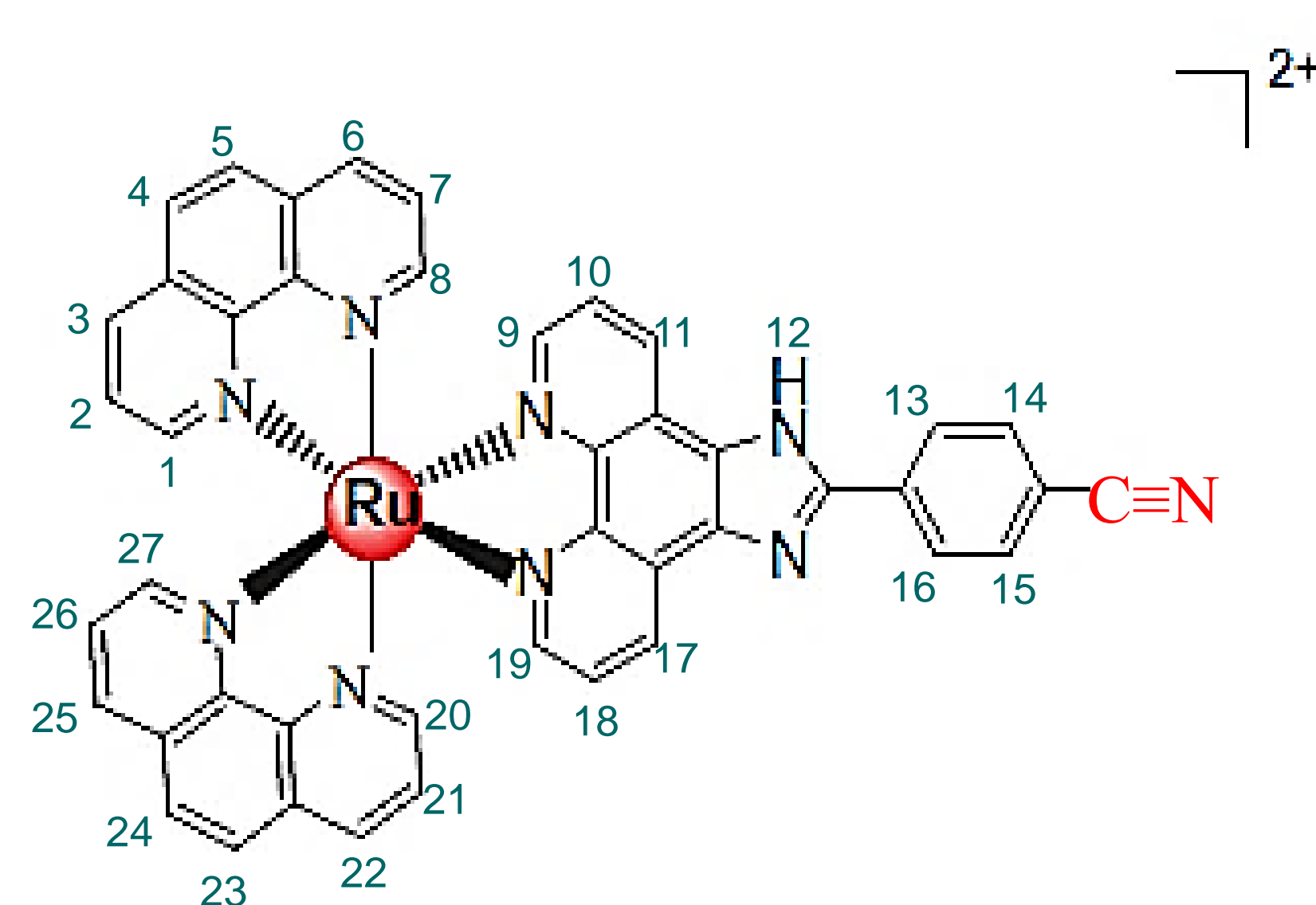


Figure 5:  $[\text{Ru}(\text{phen})_2p\text{-CPIP}]^{2+}$

## Complex Characterisation

The complexes are prepared from starting materials such as 1,10 phenanthroline, phendione,  $\text{Ru}(\text{bpy})_2\text{Cl}_2$  and  $\text{Ru}(\text{phen})_2\text{Cl}_2$  and all samples are characterised by electronic (UV/Vis, Fluorescence), vibrational (IR/Raman) and NMR ( $^1\text{H}$ ,  $^{13}\text{C}$ , COSY) spectroscopy. An example of the Raman spectrum and  $^1\text{H}$  NMR for  $\text{Ru}(\text{phen})_2p\text{-CPIP}$  is presented below in figure 6 and 8 respectively.

Figure 6: Neat Raman Spectrum of  $[\text{Ru}(\text{phen})_2p\text{-CPIP}]^{2+}$  at 785 nm.

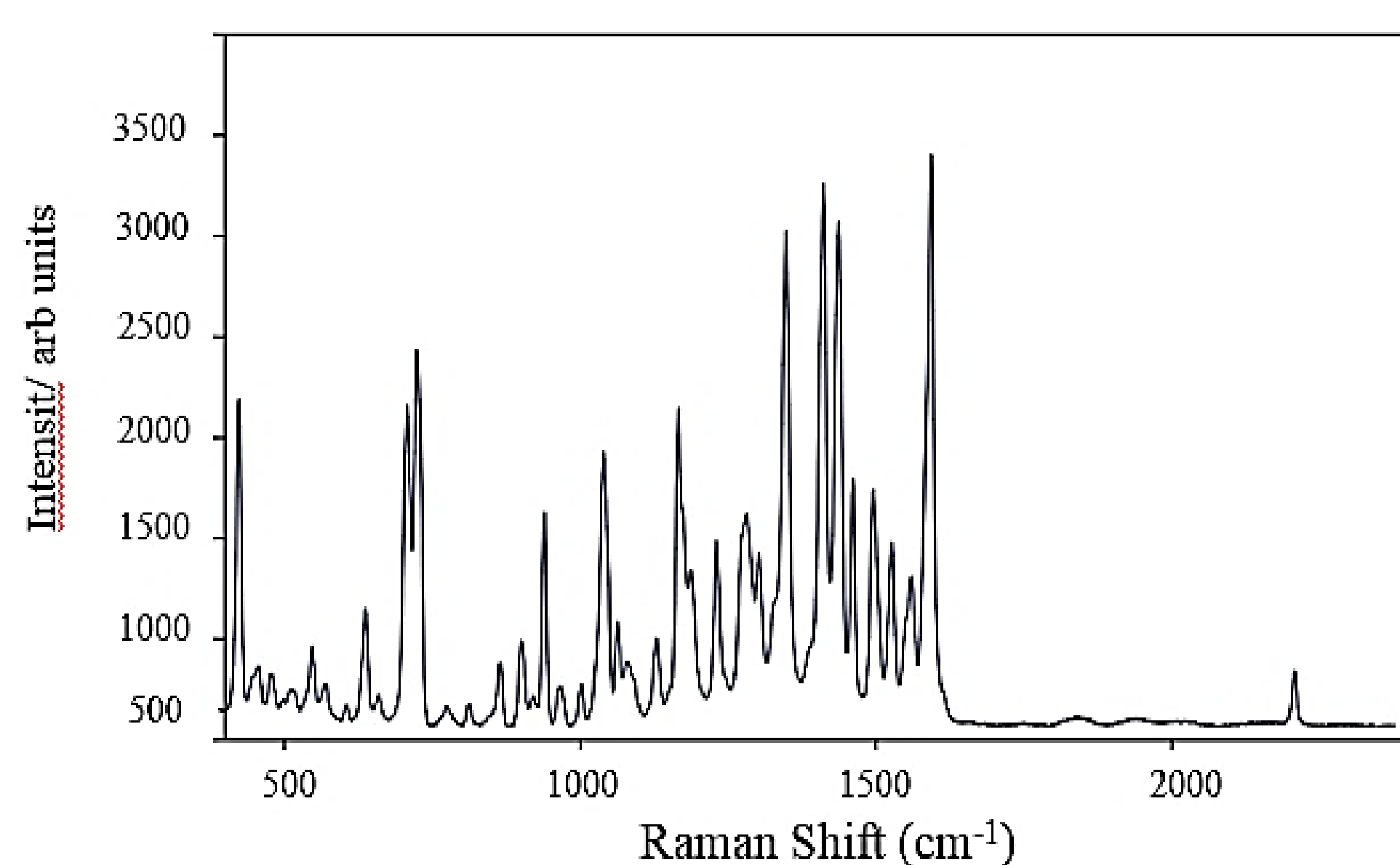


Table 1: Significant Raman Frequencies of  $[\text{Ru}(\text{phen})_2p\text{-CPIP}]^{2+}$

Assignment	Frequency ( $\text{cm}^{-1}$ )
C $\equiv$ N	2227
C=C	1610, 1544
Pyridine C=C and C=N in plane vib	1455, 1416
Imidazole ring	1354
Aromatic C=C	1321, 1295
Aromatic in plane C-H	1178
def. vib	
Aromatic out plane C-H deformation vib	962
C-H op band	736, 720

$[\text{Ru}(\text{phen})_2p\text{-CPIP}]^{2+}$  NMR Spectrum:

Samples were prepared in deuterated dimethyl sulfoxide ( $d_6\text{-DMSO}$ ) and analysed at 400 MHz.

Figure 7: COSY NMR

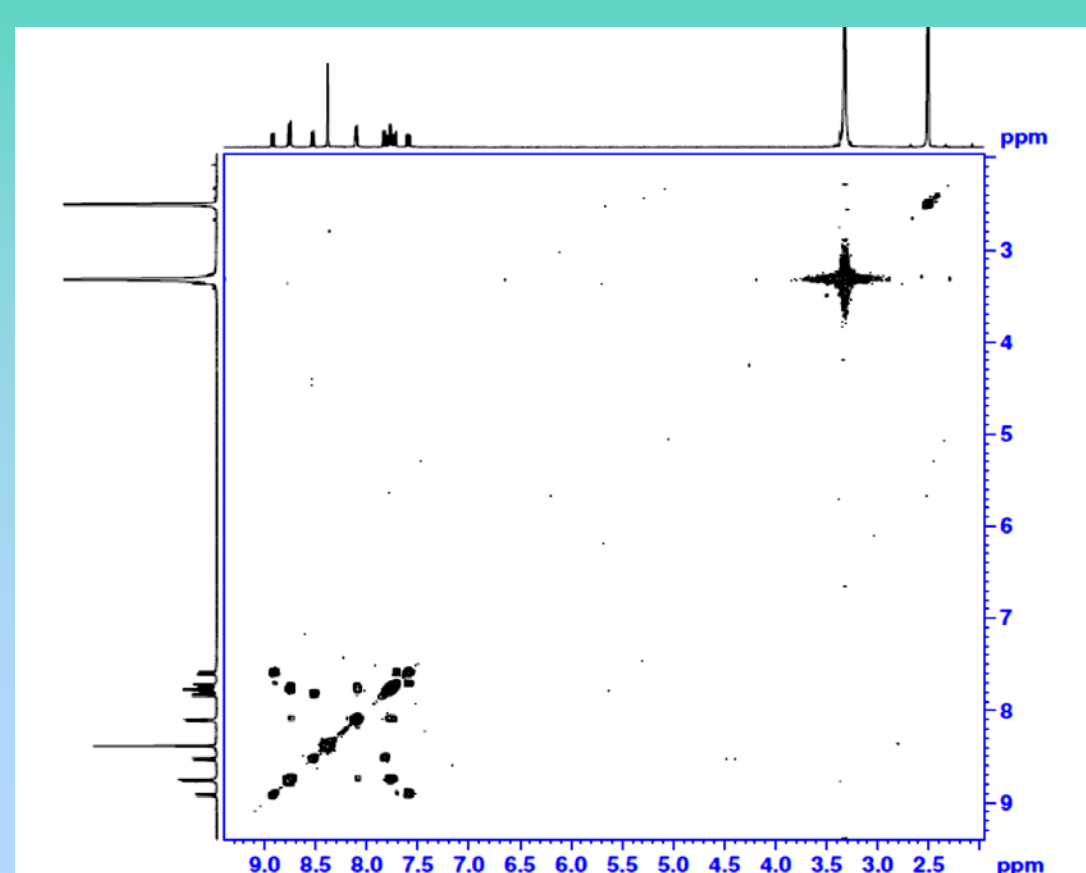
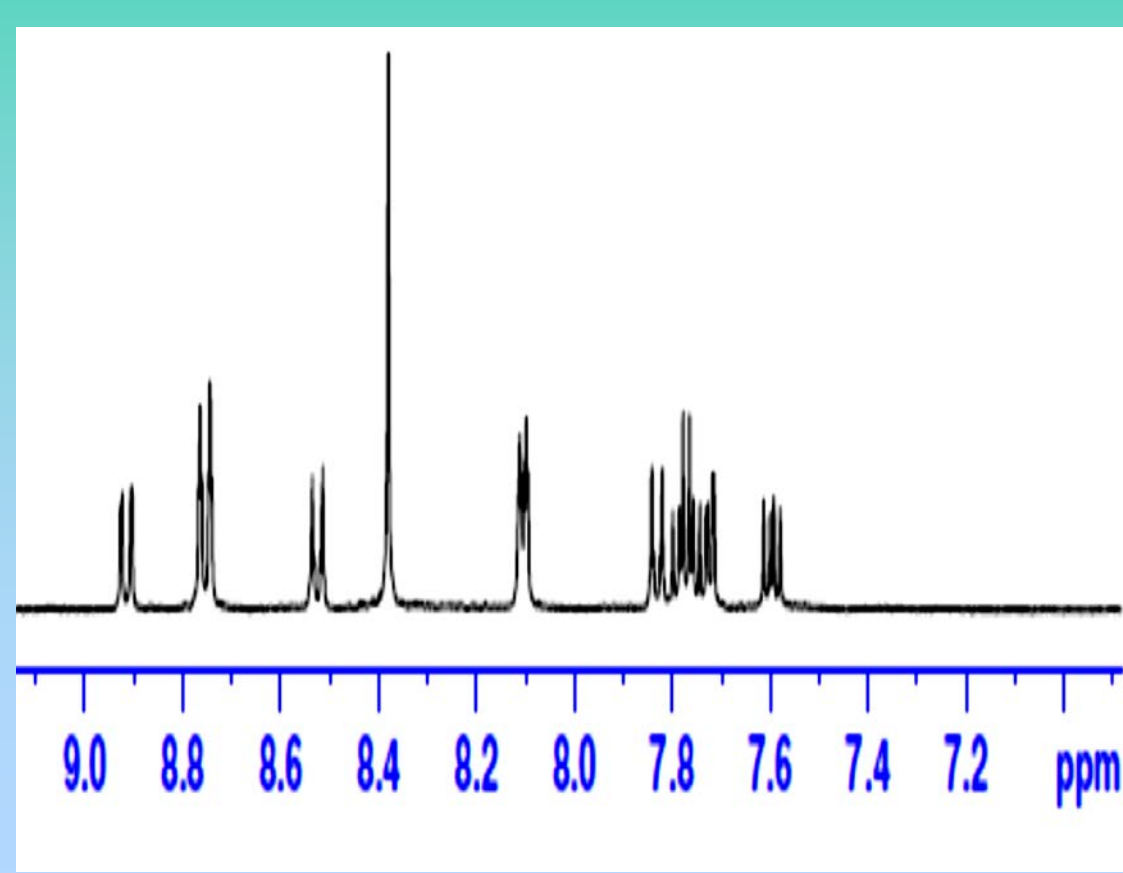


Figure 8:  $^1\text{H}$  NMR



The proton chemical shifts of  $[\text{Ru}(\text{phen})_2(\text{L})]^{2+}$  were assigned by the aid of  $^1\text{H}$ - $^1\text{H}$  COSY spectra and by comparison with structurally similar complexes.<sup>1</sup> Complexation of the phenanthroline auxiliary ligands gives a distinct proton signal, this large signal generated by the 2 aromatic protons on both phen moieties, was observed at  $\sim 8.41$  ppm in all the  $[\text{Ru}(\text{phen})_2\text{L}]^{2+}$  complexes assigned to protons at positions 4, 5, 24, 25 of the complex.<sup>5</sup>

## Biological Evaluation

- In previous studies  $[\text{Ru}(\text{phen})_2p\text{-FPIP}]^{2+}$  and  $[\text{Ru}(\text{phen})_2p\text{-CPIP}]^{2+}$  were observed to have the most effective interaction with CT-DNA of the series of Ru(II) complexes studied.<sup>5c</sup>
- They were found to have strong intercalation properties and tuneable photo-physical properties.<sup>5</sup>

## Preliminary Antibacterial Evaluation Results

Table 2: Most common bacterial strains responsible for clinical infection and contamination in health care environments worldwide.<sup>6</sup>

Enterococcus faecalis	Gram-positive
MRSA	
Escherichia Coli	Gram-negative
Pseudomonas Aeruginosa	

## Methodologies

- Evaluation of Antibacterial Activity by 96 well-plate technique.

Figure 9: Preliminary Antibacterial Activity of Phendione.

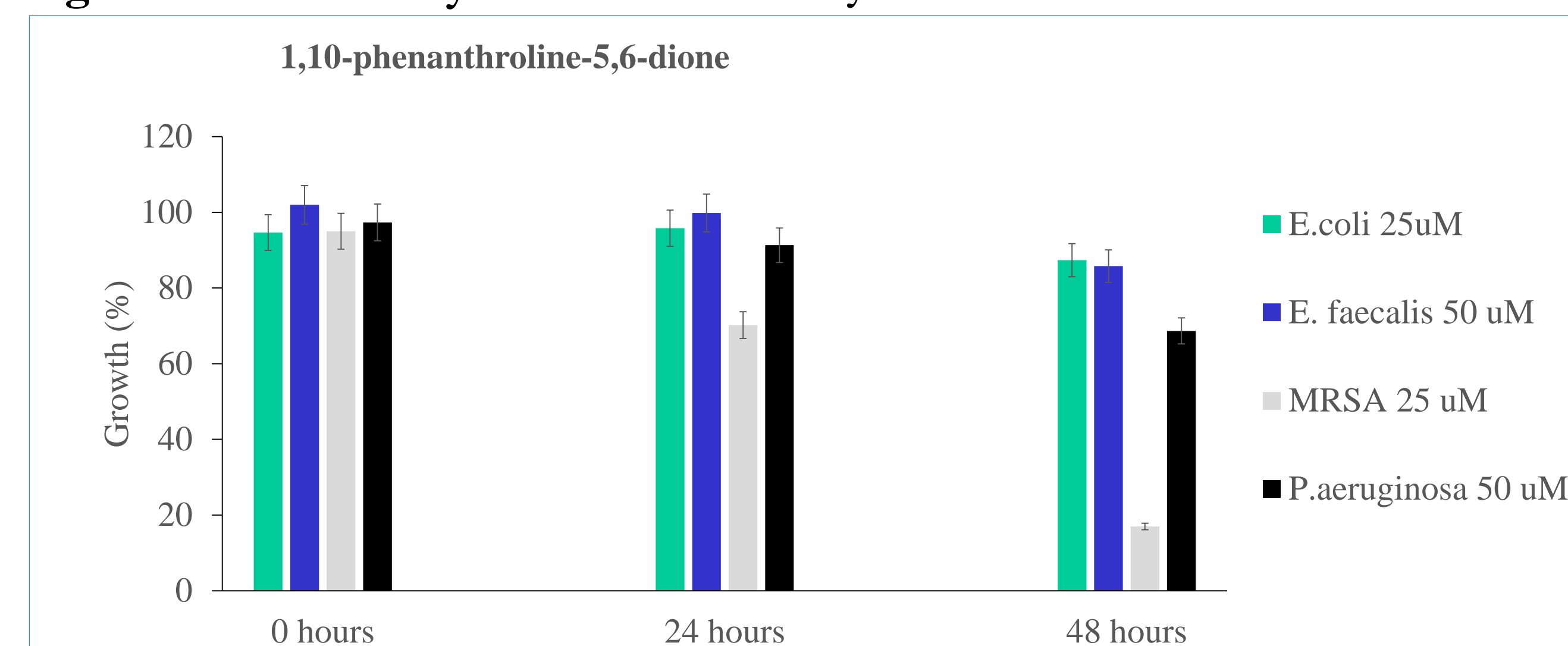
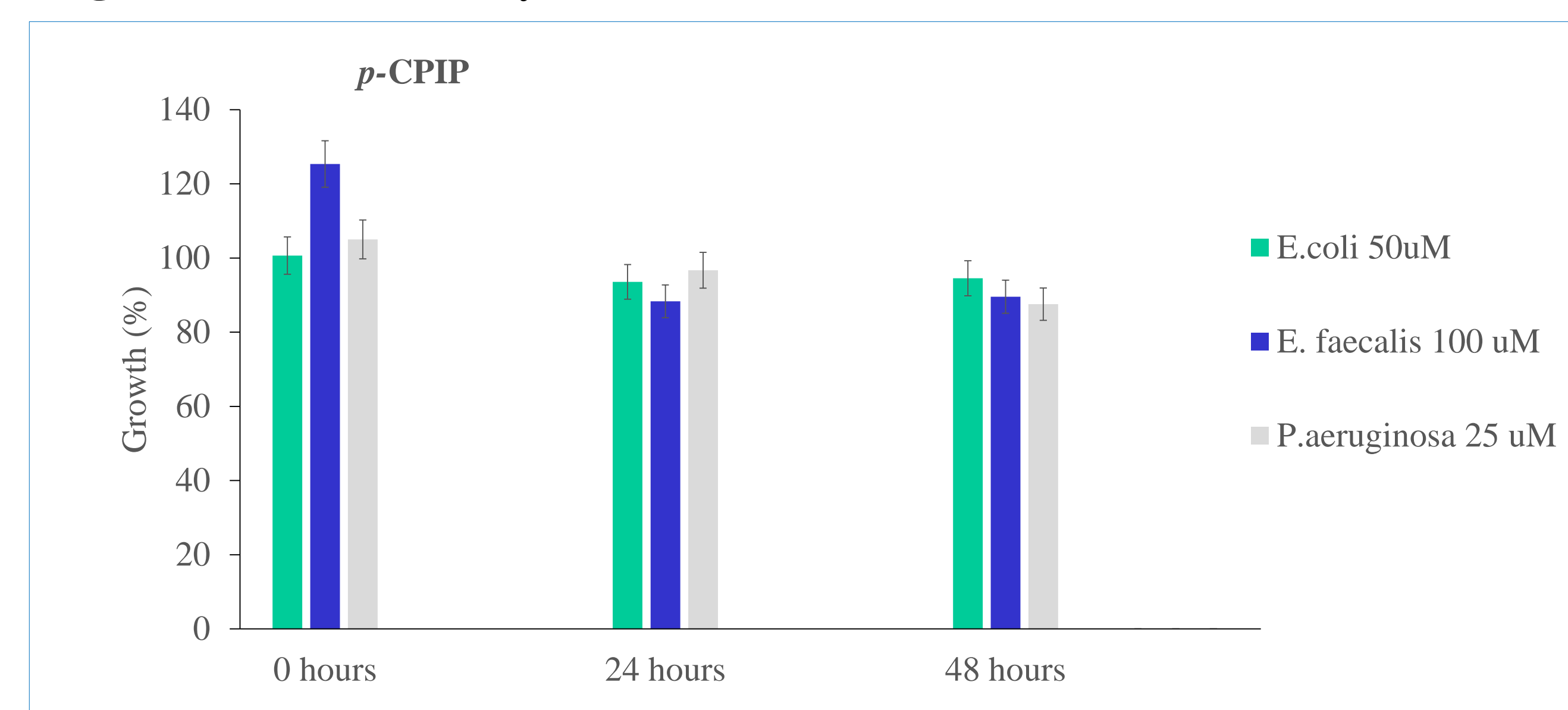


Figure 10: Preliminary Antibacterial Activity of CPIP.



## Conclusion

To date phendione has shown the most antibacterial effectiveness for the gram-positive and gram-negative bacterial strains tested at different concentrations. The CPIP ligand shows effectiveness at higher concentrations than the phendione on the same bacterial strain studied. However, it shown ineffective against MRSA.

The ruthenium complex tested has shown certain efficiency to *E.Coli* and *P. Aeruginosa*, as preliminary studies, it can be considered for further testing as a novel antibacterial therapeutic for different strains of bacteria. Further studies correlating different novel antibacterial therapeutics based on ruthenium compounds at varying concentrations will be continued against different bacterial strains in the future.

## Aknowlegments

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