(12) PATENT APPLICATION PUBLICATION

(19) INDIA

(86) International Application

(87) International Publication

(62) Divisional to Application

(61) Patent of Addition to

Filing Date

Application Number

Filing Date

Filing Date

No

No

Number

(22) Date of filing of Application: 10/01/2024

 $(51)\ International\ classification \\ \frac{(51)\ International\ classification}{(57)\ C07F1/08,\ C07F15/02,\ C07F15/04,\ C07F15/06}$

: NA

·NA

:NA

:NA

(21) Application No.202441001810 A

(43) Publication Date: 09/02/2024

(54) Title of the invention : BERBERINE-METAL COMPLEXES AS PROMISING ANTIBACTERIAL AND ANTIFUNGAL AGENTS TO FIGHT DRUG RESISTANCE

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(57) Abstract :

ABSTRACT In this research, a series of experiments was conducted, involved the synthesis and characterization analysis of complexes formed between Berberine and various metals. These compounds were characterized using techniques such as IR, NMR, MASS, and P-XRD to evaluate their binding affinity. We also assessed their efficacy in inhibiting a range of microorganisms, including gram-negative bacteria (E. coli, P. aeruginosa), gram-positive bacteria (B. cereus, S. mutans), and a fungal organism (C. albicans), while determining their respective IC50 values. Furthermore, we performed docking experiments using ten synthesized compounds with a specific protein (PDB ID: 5C5H,7V67). Among these compounds, the Berberine-Cu Complex (b1) demonstrated the most favorable binding affinity with proteins 5C5H (associated to gram negative bacterial activity) and 7V67 (associated to antifungal activity), achieving scores of -9.0 kcal/mol and -9.9 kcal/mol, respectively. It is confirmed that this study will also serve as a valuable foundation for the development of novel antimicrobial medications.

No. of Pages: 21 No. of Claims: 1