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Investigations on the Cytotoxicity and Antimicrobial Activities of Terezine E and 14-Hydroxyterezine D

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Abstract : Secondary metabolites produced by endophytes are an excellent source of biologically active compounds. In our current study, we evaluated terezine E and 14-hydroxyterezine D for binding to the active site of histone deacetylase (PDB ID: 4CBT) and matrix metalloproteinase 9 (PDB ID: 4H3X) by molecular docking using AutoDock Vina software after having tested their cytotoxic activities on three cell lines (human ductal breast epithelial tumor cells (T47D)-HCC1937), human hepatocarcinoma cell line (HepG2)-HB8065), and human colorectal carcinoma cells (HCT-116)-TCP1006, purchased from ATCC, USA)). Additionally, their antimicrobial activities were investigated, and their minimum inhibitory concentration (MIC) values were determined against P. notatum and S. aureus by the broth microdilution method. Higher cytotoxicity was observed for terezine E against all tested cell lines compared to 14-hydroxyterezine D. Molecular docking results supported the high cytotoxicity of terezine E and showed higher binding affinity with 4CBT with an energy score of 9 kcal/mol. Terezine E showed higher antibacterial and antifungal activities than 14-hydroxyrerezine D: MIC values were 15.45 and 21.73 mg/mL against S. aureus and 8.61 and 11.54 mg/mL against P. notatum, respectively

Keywords : Terezine E, 14-Hydroxyterezine D, cytotoxicity, antimicrobial activity, molecular docking
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