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A COMPUTATIONAL APPROACH TO IDENTIFY BETA-LACTAM-LIKE COMPOUNDS FROM PHYTOCHEMICALS

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Antimicrobial resistance (AMR) is one of this century's most severe global health problems. It has been estimated that AMR is directly responsible for 700,000 deaths annually, which is predicted to be 10 million by 2050. Present antibiotics are failing due to various reasons while phytochemicals are gaining attention due to their favorable attributes as antimicrobials. Many studies have shown the importance of applying Computational Biology to Microbiology. In this context, the KNIME (Konstanz Information Miner) analytics platform was used for our analysis. The primary goals of this research were to develop a KNIME workflow using a Machine Learning approach to discover potential compounds with beta-lactam properties from a set of phytochemicals and to use a 96-well plate assay to screen such candidate compounds biochemically. Compound data were acquired for beta-lactams, non-antibiotic drugs and phytochemicals from ChEMBL. Cells of molecule string column were converted into SMILES (Simplified Molecular Input Line Entry System). RDKit molecule column was generated from SMILES. Fingerprints were generated, and data was prepared for Machine Learning. Machine Learning algorithms were used to train the filtered ChEMBL dataset to discriminate between active and inactive compounds. After comparing the structural similarities, a set of phytochemicals (decanoic acid, alpha-pinene) was identified as hits for beta-lactams with more than 85% overall accuracy. Decanoic acid was screened biochemically. A slight growth inhibition was observed with increasing decanoic acid concentration from 100-700 μgmL^{-1}. The developed KNIME workflow can identify possible beta-lactam-like compounds from a set of phytochemicals. Ninety-six well plate assay is a significant method to screen a large number of hits simultaneously. In conclusion, the intended KNIME workflow has been successfully developed and seven phytochemicals as hits for beta-lactams were found. As future directions other candidate compounds will be screened and further analyzed.

Keywords: Antibiotics, Antimicrobial resistance, KNIME, Machine Learning, 96-well plate assay