



Synthesis and QSAR Analysis of Oxazolo/thiazolo Pyrimidine Derivatives as Potential Antibacterial Agents

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SUMMARY. Development of new antibacterial agents is increasingly important due to the resistance of microbes to the known antibacterial drugs. A series of benzylidene oxazolo/thiazolo (3,2-a)-pyrimidine-6-carboxamides were synthesized by condensing 2-oxo/thio-1,2,3,4-tetrahydropyrimidine carboxamides with various aromatic aldehydes. The structures of newly synthesized compounds were characterized by IR and NMR spectral data. All the compounds were screened for their antibacterial activity against Gram-positive and Gram-negative bacteria and MIC values were determined by serial dilution method. The 2D-QSAR studies were performed on VLife MDS software. QSAR equation revealed that selected physicochemical parameters such as Alignment Independent, Electrostatic and 2PathCount have correlation with antibacterial activity. Among synthesized benzylidene oxazolo or thiazolo (3,2-a) pyrimidine-6-carboxamide derivatives, compounds containing electron withdrawing polar group at para position of 5-phenyl ring and electron withdrawing non-polar group at para position of 2-benzylidene moiety of thiazolopyrimidine nucleus are better antibacterials.

KEY WORDS: Antibacterial activity, Carboxamide, Oxazolopyrimidine, QSAR, Thiazolopyrimidine.

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