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New Microbiological and Pharmacokinetic models

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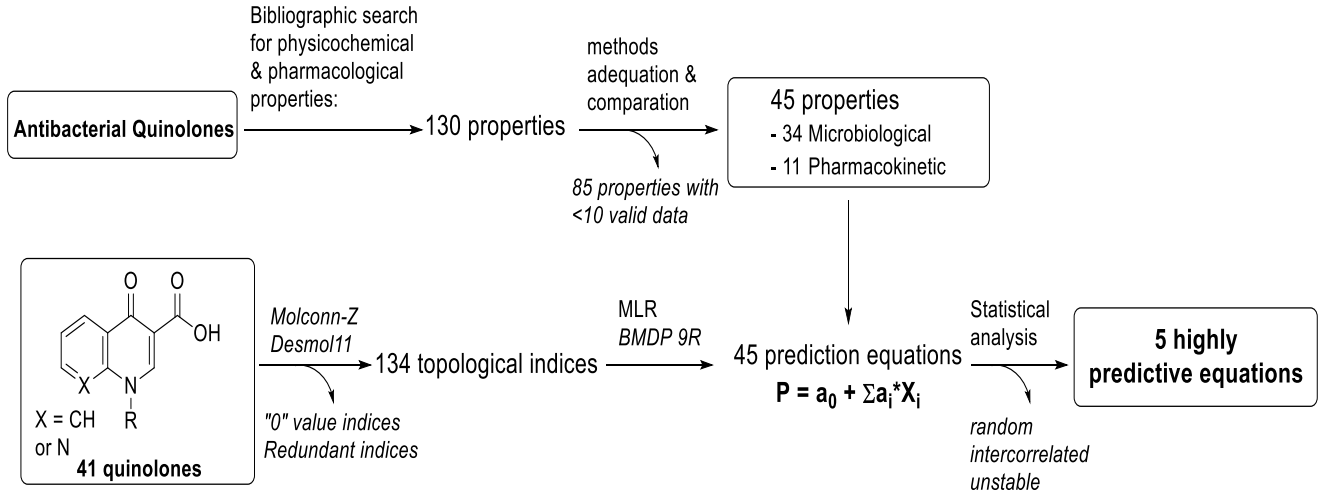
Abstract. Abstract: In this paper, a multilinear regression (MLR) analysis has been carried out in order to accurately predict physicochemical properties and biological activities on a group of antibacterial quinolones by means of a set of structural descriptors called topological indices. The aim of this work is to develop prediction equations for these properties after collecting the maximum number of data from the literature on antibacterial quinolones. The five regression functions selected by presenting the best combination of various statistical parameters, subsequently validated by means of internal validation (intercorrelation, Y-randomization and leave-one-out cross-validation tests), allowed the reliable prediction of minimum inhibitory concentration 50 versus *Staphylococcus aureus* (MIC50Sa), *Streptococcus pyogenes* (MIC50Spy) and *Bacteroides fragilis* (MIC50Bf), mean residence time (MRT) after oral administration and volume of distribution (V_D). We conclude that the combination of molecular topology methods and MLR provides an excellent tool for the prediction of pharmacological properties.

Graphical Abstract



Keywords: molecular topology, multilinear regression (MLR), molecular connectivity, topological indices, quinolones, QSAR.

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