



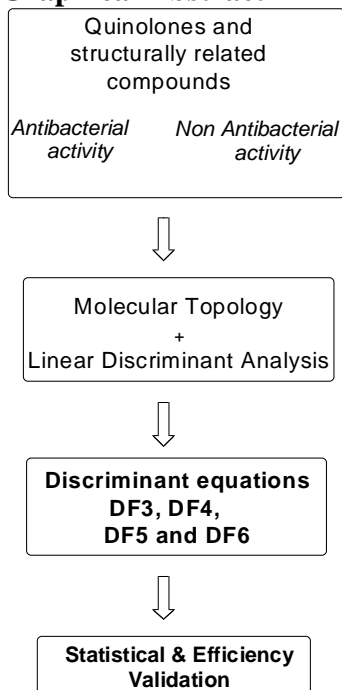
## Discriminant Equations for the Search of New Antibacterial Drugs

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### Graphical Abstract



### Abstract

*In this study, molecular topology was used to develop several discriminant equations capable of classifying compounds according to their antibacterial activity.*

*Topological indices were used as structural descriptors and their relation to antibacterial activity was determined by applying linear discriminant analysis (LDA) on a group of quinolones and quinolone-like compounds.*

*Four extra equations were constructed, named DF3, DF4, DF5 and DF6 (DF1 and DF2 were built in a previous study), all with good statistical parameters such as Fisher-Snedecor  $F$  ( $> 25$  in all cases), Wilk's lambda ( $< 0.36$  in all cases) and percentage of correct classification ( $> 80\%$  in all cases), which allows a reliable extrapolation prediction of antibacterial activity in any organic compound.*

*The results obtained clearly reveal the high efficiency of combining molecular topology with LDA for the prediction of antibacterial activity.*

**References** (*mandatory*)

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