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Discriminant Equations for the Search of New Anti-MRSA Drugs

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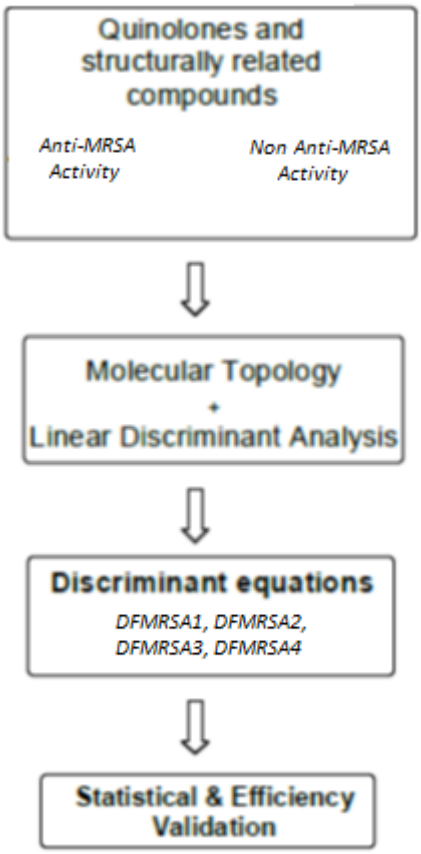
Graphical Abstract	**Abstract.**
	The variability of methicillin-resistant Staphylococcus aureus (MRSA), its rapid adaptive response against environmental changes, and its continued acquisition of antibiotic resistance determinants, have made it a habitual resident of hospitals, where it causes a problem of multidrug resistance. *In this study, molecular topology was used to develop several discriminant equations capable of classifying compounds according to their anti-MRSA activity.* *Topological indices were used as structural*



descriptors and their relationship to anti-MRSA activity was determined by applying linear discriminant analysis (LDA) on a group of quinolones and quinolone-like compounds.

Four extra equations were constructed, named DFMRSA1, DFMRSA2, DFMRSA3 and DFMRSA4 (DFMRSA was built in a previous study), all with good statistical parameters such as Fisher-Snedecor F (> 68 in all cases), Wilk's lambda (< 0.13 in all cases) and percentage of correct classification (> 94 % 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 anti-MRSA activity.

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