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Two- and Three-Dimensional Quantitative Structure-Activity Relationships Studies on a Series of Diuretics

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***SUMMAARY*. Diuretics are an attractive class of drugs for the treatment of various disorders and in combination with some cardiovascular drugs. In the present work, 2D and 3D quantitative structure-activity relationship studies have been conducted on a series of diuretics. Significant correlation coefficients (r^2 = 0.81 and q^2 = 0.65, r^2 = 0.91 and q^2 = 0.85) were obtained, indicating potential of the models generated for untested compounds. The models were then used to predict the potency of an external test set, and the predicted values obtained from the 2D and 3D models were in good agreement with the experimental results. The final QSAR models, along with the information obtained from 3D steric and electrostatic contour maps and 2D contributions should be useful for the design of diuretics having improved potency.**

KEY WORDS: Diuretics, Drug design, QSAR.

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