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Quantitative Structure-Activity Relationship (QSAR) Model Review

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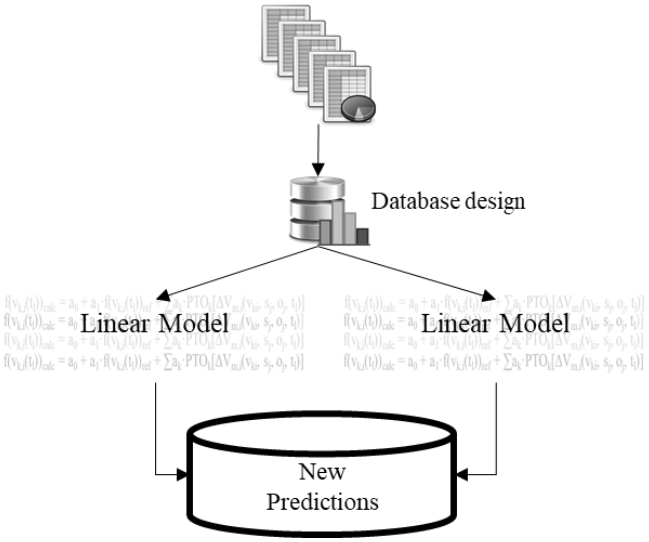
Graphical Abstract



Abstract.

The Quantitative Structure-Activity Relationship (QSAR) models are a very useful tool in the design of new chemical compounds. The QSAR methods are based on the assumption that the activity of a certain chemical compound is related to its structure.

Two types of QSAR analysis are summarized in this review: Linear Regression model (LR) and Linear Discriminant Analysis model (LDA).

Introduction

The Quantitative Structure-Activity Relationship (QSAR) models are a very useful tool in the design of new chemical compounds. The QSAR methods are based on the assumption that the activity of a certain chemical compound is related to its structure[1]. More precisely, this approach says that the activity, or the property, is related to the chemical structure through a certain mathematical algorithm, or rule. QSAR models are also called in silico methods, which actually refer to a somehow broader set of methods.

The number of published works in the last years has increased, this can be seen in **Figure 1**.

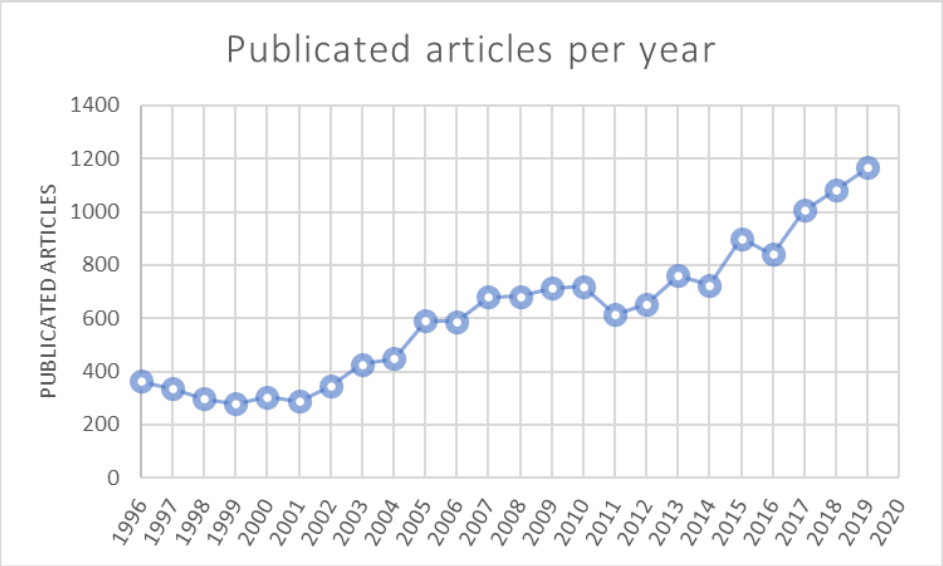


Figure 1. Review of published papers since 1996 with "QSAR" as keyword.

A QSAR method tries to find out a relationship between the response of activity or property, the dependent variable $f(v_{ij})_{calc}$ and the alterations in value of physical-chemical or structural attributes as change descriptors, **Equation 1**.

$$f(v_{ij})_{calc} = a_0 + a_1 D_1 + a_2 D_2 + \cdots + a_n D_n \quad (1)$$

Two types of QSAR analysis are summarized in this review: Linear Regression model[2] (LR) and Linear Discriminant Analysis model (LDA).

Materials and Methods

The main difference between these two techniques is that regression analysis deals with a continuous dependent variable, while discriminant analysis must have a discrete dependent variable.

The model generated with LDA method is a generalization of Fisher's linear discriminant analysis. It is a method used in statistics, pattern recognition, and machine learning to find a linear combination of features that characterize or separate two or more kinds of objects or events. The resulting combination can be used as a linear classifier. This type of model is used to predict bankruptcy[3], image recognition[4], marketing[5], medicinal studies[1], earth science[6]…

LR model is one of the most frequently used statistical methods and its used to predict a numeric response variable based on one or more numeric explanatory variables. Prediction is most straightforward when there is a straight-line relationship between a single explanatory variable and numeric response variable. This method is more appropriated when both variables are numeric. This model is a good option when the database has a homogeneous distribution, so it can be said that it has a homoscedastic distribution. The most common locations for these models are trend lines, medicine, informatics…

References

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