

Abstract

Using Machine Learning-Based Hierarchical Support Vector Regression Approach to Predict Skin Permeability [†]

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Abstract: Skin is the largest organ in the human body, and it works as the natural barrier against the external environment. Furthermore, topical and transdermal drug delivery has emerged as a new effective and safer administration choice. A variety of in vitro, in vivo, and ex vivo assays have been adopted to evaluate the retention of the drug in the skin layers and the skin permeability, in which the ex vivo excised human skin has been considered as the gold standard to assess the skin penetration despite its potential for ethical issues. In this study, the novel machine learning-based hierarchical support vector regression (HSVR) was adopted to generate a nonlinear quantitative structure–activity relationship (QSAR) model, which can predict the K_p values based on the ex vivo human skin permeability data. The HSVR model showed a consistent performance with the experimental data and among the training set, test set, outlier set, and mock test, which was designated to mimic the real challenges. In addition, the HSVR exhibited a better prediction performance than the classical partial least squares (PLS) did. Thus, it can be concluded that the novel HSVR model can be utilized to facilitate the assessment of the skin permeability of the novel compounds in drug discovery.

Keywords: skin permeability; ex vivo excised human skin; hierarchical support vector regression (HSVR); quantitative structure–activity relationship (QSAR); partial least square (PLS)

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