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Predicting hydrolyzability using logistic regression analyses and regularization techniques

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It is significant to estimate the environmental fates of chemical substances which are emitted from factories or as residential wastes. Especially, since hydrolysis plays a main role with regard to chemical substance degradation in the environment, hydrolyzability of such chemicals have to be revealed. However, experimentally obtaining the information is time-consuming. Thus, we tried to predict the hydrolyzability of esters and related compounds using logistic regressions and regularization methods. The hydrolyzability data of 143 chemicals, which were extracted from literatures, were used for these analyses. These chemicals were classified into two categories, 'stable' and 'hydrolizable', according to their half-life periods. They were also classified into four groups, all chemicals (143), esters (73), amides, and others. In this study, the former two groups were analysed. 88 chemical descriptors were prepared for predicting the hydrolyzability. All the datasets were divided into training (3/4) and test (1/4) sets. Lasso was used as a regularization method. We built the model equation by two techniques using only training data sets. As the results of the analyses, training data were perfectly predicted in the case of esters, and sufficient results were obtained in the case of all chemicals. Even in the case of test data sets, satisfactory results were obtained.

Biography

Tatsuya Takagi has completed his PhD from Osaka University. At the same time, he had been as an Assistant Professor of School of Pharmaceutical Sciences, Osaka University for 5 years. Then, since 1993, he had worked for the Genome Information Research Center, Osaka University as an Associate Professor until he became a Professor of Graduate School of Pharmaceutical Sciences, Osaka University in 1998. He has published more than 100 papers in reputed journals and serving as Chairman of Division of Structure-Activity Relationship of the Pharmaceutical Society of Japan.

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