

クラスター分析による構造類似性と薬効・薬理情報の相関性の検討と副作用予測

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Study of Correlation Between Structural Similarities by Cluster Analysis and Efficacy/Pharmacology Information, and Prediction of Adverse Drug Reaction

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Abstract

Efficacy and pharmacological actions of drugs can be described to be the outcomes of their actions based on their structures that fit to various drug receptors in vivo, and drugs are hypothesized to have a similar pharmacological action if they share a similar structure. Studying an event with actual establishment of the above hypothesis requires a method for comparing objective structures of drugs with a classification of information on their actions, etc. Therefore we performed correlative evaluation of a structure classification obtained from a cluster analysis based on the drugs structural similarities and a classification of drug information such as known efficacy or pharmacological action. In this study, we applied a cluster analysis to 1,191 items of drugs with their known information classified, and determined the pharmacological action that represented each group from the information of the drugs that belonged to the group according to their structural similarities. We then further examined whether the action representing the group could be the common information shared among all the drugs in the group, and attempted to develop conditions and application methods required for a cluster analysis. Further, we analyzed the result and studied whether the drug information including known pharmacological actions could be described from their structural similarities. We found that the drug structures classified by a cluster analysis are correlated with the drug information classification, and ascertained that onset of adverse drug reaction can be described using analysis of a cluster.

Key words: Package Inserts, Structure Similarity Search, DI, Cluster Analysis