Abstract

***Anal. Sci.*, 17** [suppl.**]**, i467-i470 (2002)

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Recognition of relationships between mass spectral data and chemical structures by multivariate data analysis.

Chemometric methods based on multivariate data analysis can be successfully applied for investigations of relationships between mass spectra and chemical structures as well as for the development of classifiers that recognize presence or absence of substructures.

An essential step is an appropriate transformation of the original peak height data into a set of spectral features.

Examples demonstrate the use of principal component analysis and KNN classification for the determination of the number of double bond equivalents of aliphatic/alicyclic ketones, and the recognition of an acetyl substructure.

Mass spectra classification together with automatic isomer generation are applied for systematic structure elucidation, shown by an example for a compound with molecular formula $C_{10}H_{12}O_2$.