Abstract

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Spectral similarity versus structural similarity: mass spectrometry.

A recently described method [Anal. Chim. Acta 490 (2003) 313] for the evaluation of spectral similarity searches has been applied to low resolution mass spectra.

Aim of the method is to measure the similarity between the chemical structures of query compounds and the chemical structures of the found reference compounds (hits). A high structural similarity is desirable if the query is not present in the spectral library.

Similarity of chemical structures has been measured by the Tanimoto index, calculated from 1365 binary substructure descriptors. The method has been applied to sets of 200–10,000 hitlists obtained with different search methods from a database containing 106,955 compounds. Hitlists with highest structure information have been obtained by using a similarity measure based on the correlation coefficient computed either from spectral features, or from the cubic root of peak intensities for masses up to 200.

Frequency distributions of spectral and structural similarities have been investigated and a threshold for the spectral similarity has been derived that in general yields hitlists with structures that are very similar to the query structure.

An example compares different search methods.