Abstract

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Spectral similarity versus structural similarity: infrared spectroscopy.

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

Similarity of chemical structures was measured by the Tanimoto index, calculated from 1365 binary substructure descriptors.

The method has been applied to several 1000 hitlists from searches in an infrared (IR) spectra database containing 13,484 compounds. Hitlists with highest structure information were obtained using a similarity measure based on the correlation coefficient computed from mean centered absorbance units.

Frequency distributions of spectral and structural similarities have been investigated and a threshold for the spectral similarity has been derived that in general gives hitlists exhibiting significant chemical structure similarities with the query.