

Abstract

Asian Chemistry Letters, **13**, 195-200 (2009)

Penchev P.N., Andreev G.N., Varmuza K.:

Computer-assisted structure elucidation of organic compounds by infrared spectroscopy

The joint application of several chemometric methods for infrared spectra interpretation/classification is described.

The methods are implemented in several programs working under MS-DOS and Windows environment. They include: 1) seven routines for searching in spectral libraries; 2) binary classification with artificial neural networks, linear discriminant functions and expert-knowledge classifiers; 3) processing of library search results (a hitlist) with the concept of maximum common substructure and with a set of k-nearest neighbor classifiers.

As an illustration of the structure elucidation process an example is given.