PATTERN EXPERT
Solutions for Pattern Recognition

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Program Information

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Spectroscopy allows for a safe identification of chemical compounds. However, analyzing highly complex spectra of samples, which represent mixtures - like biological samples or complex chemicals - is much more difficult.
The software “PATTERN EXPERT airspect” (**A**daptive **I**nformation Extraction and **R**esearch System for **Spect**roscopy) yields a clear classification even for spectra of complex mixtures with respect to a given problem.
“PATTERN EXPERT airspect” is based on powerful algorithms from neural information processing and pattern recognition.

Numerous Applications for Science and Technology

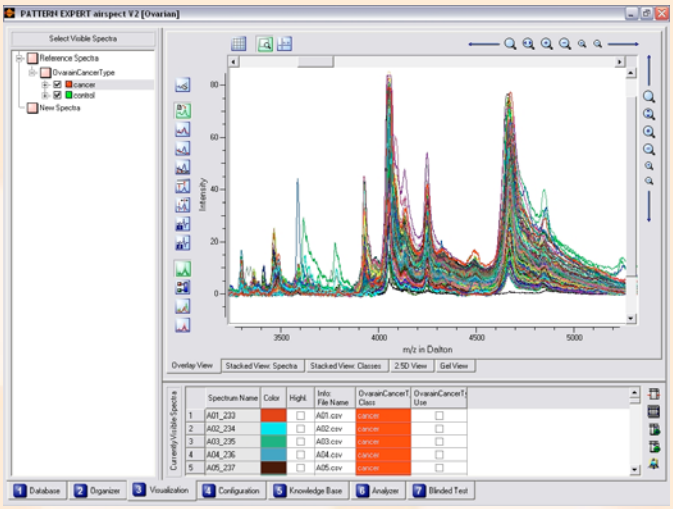
The software has been developed in collaboration with the Forensic Science Institute of the “Bundeskriminalamt” (the German central police agency). There, it is used for identifying mass product samples. Building up collections of spectra is a common method in the material and life sciences, in chemometry and quality control. airspect helps to extract the knowledge contained in these collections in an optimal manner and to make it accessible to a large number of users.

Simple Operation

The program airspect can be used to construct and train so-called “knowledge bases” in a fully automatic manner. No previous experience or knowledge is needed, for instance from the fields of signal processing or neural information processing. The user just needs to assign the individual spectra of his collection to the desired classes, which can be done in a very easy and efficient way.
The training process takes, depending on the difficulty of the task, between a few seconds to several hours.

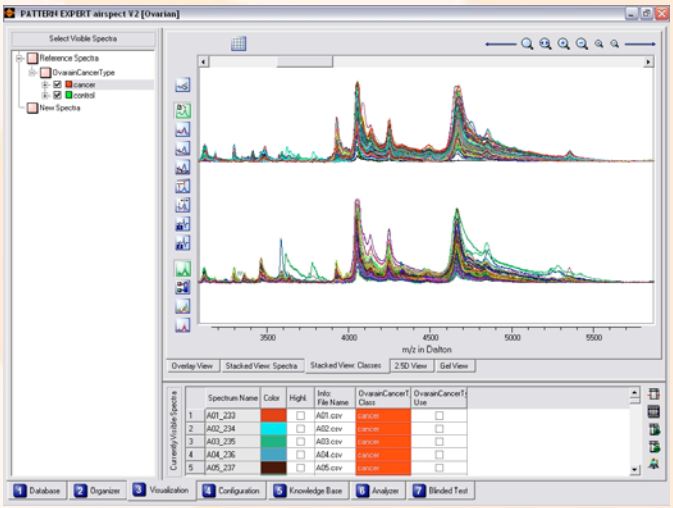
After training, the system is ready for classifying new unknown spectra.

The system has been tested with large collections of more than 2000 spectra in over 25 classes with great success.



Visualizations for Detailed Analysis

For data analysis by the human user the software offers clear visualizations, for example diagrams of preprocessed spectra or their derivatives, diagrams of several spectra stacked one above the other, or the mean and standard deviation curves of all spectra belonging to one class.



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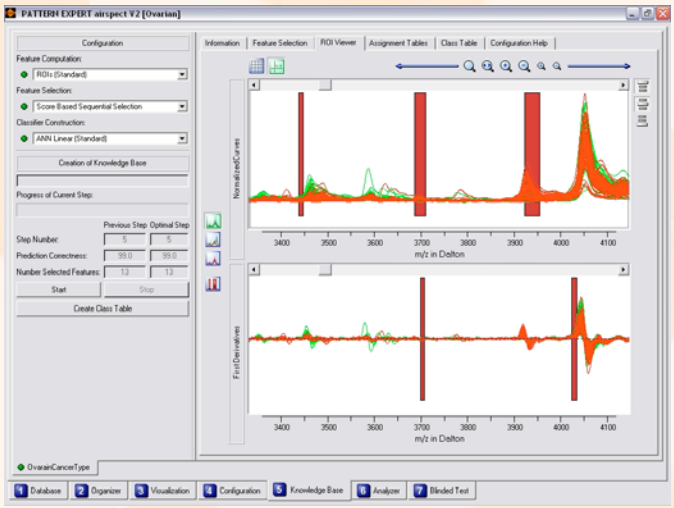
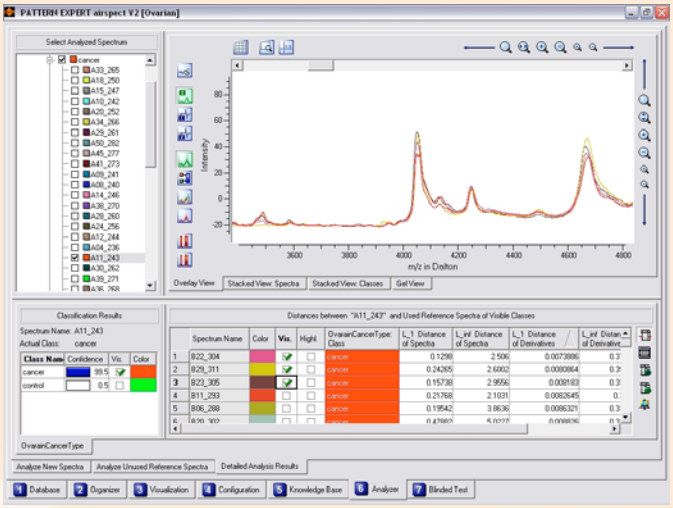
Extensive Analysis Tools for the Classification System

For construction and training of the “knowledge bases”, the user selects from several methods. Depending on the current task, one is able to choose the best procedure possible.
When the training process has been completed, there are various tools available for analyzing the resulting classification system. For example, the spectral ranges, which have been found to be relevant for the given problem, can be displayed in a diagram or table.



High Accuracy at Retrieval of Matching Reference Spectra

In addition, the software offers various powerful tools for analyzing the individual spectra of unknown samples.
The unknown spectra can be classified or compared with reference spectra from the database. The algorithms for “knowledge base” training are used at the same time as an intelligent means for generating well-adapted distance measures, which can be used to find the “nearest” reference spectra for a given unknown spectrum.
As experience shows, when trying to retrieve similar reference spectra from a database, airspect finds the actually best matches immediately.



Technical Characteristics:

The software is presently able to import infrared spectra in JCAMP-DX or ASCII format. Additional input formats can be delivered on demand.

Program Characteristics:

- Simple and intuitive operation.
- Fully automatic preprocessing (removal of jump discontinuities, baseline correction, rescaling).
- Visualization of spectra: original curves, intermediate and final results of preprocessing, 1st and 2nd derivatives, 1 dim., 2.5 dim., “Gel View”.
- Fully automatic generation of characteristic features for classification.
- Efficient assignment of spectra to classes by a table or by directory structure.
- Tabular presentation of learning and classification results.
- Optional use of additional user-defined information for classification.
- Efficient control of the algorithms for “knowledge base” construction and training via scripts (additional scripts for special tasks available on demand).

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