

## **Chemometrics and Spectroscopy Problems Solving by Chemical Portal**

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### **Abstract**

The possibilities of the [www.e-chemia.pl](http://www.e-chemia.pl) portal application to teaching the basics of spectroscopy and the possibilities of spectral data processing by means of advanced chemometric methods were presented. Lesson modules concern IR, Raman, UV-Vis,  $^1\text{H}$ NMR,  $^{13}\text{C}$  NMR and MS spectroscopies. The chosen chemometric methods: linear learning machine, k-Nearest Neighbour, artificial neural network and cluster analysis are used for spectrum classification and type-of-compound prediction. The didactic materials that were worked out are used by the students of the Faculty of Chemistry, Rzeszów University of Technology (Poland) as a learning aid for subjects that require the skill of molecular spectrum interpretation as well as in chemometric and computer chemistry teaching.

### **Keywords**

blended learning, chemometrics, spectroscopy

### **INTRODUCTION**

Spectroscopy is an exquisite analytical technique and its application in our everyday life is widespread. Infrared, ultraviolet- visible, NMR and MS spectroscopies are integral parts of modern chemistry and for these reasons these analytical methods should be incorporated into an educational program not only for chemistry students but also for students of other nature sciences. The importance of spectral methods for teaching chemistry students is pointed out by numerous publications and conferences devoted to this topic. In modern chemistry teaching, so also in spectroscopy, more and more attention is paid to the use of computer technologies. This is evidenced by the activities of such organizations as The Committee of Computers in Chemical Education, an appointed committee of the division of Chemical Education of the American Chemical Society whose mission is to "encourage and support the development, assessment and use of computing technologies in chemical education" (DivCHED CCCE, 2012).

There are more and more teaching tools aiding teaching and learning spectroscopy available on CD-ROMs or through the WEB (Blackman, 2012; Bradley et al., 2009; Dębska & Guzowska-Świder, 2007; Hornak, 2012; King & Wong, 2012; 2012; Sauriol, 2012; Spectroscopy n.d.; SPINUS-WEB, 2012), which is a really convenient way of spreading information. There is access to electronic versions of conventional, printed textbooks, slides and texts of lectures delivered, didactic materials describing laboratory exercise techniques or solving problems, collections of real spectra, recorded lectures or video clips that show practical aspects of the spectroscopic

techniques. However, students find interactive software and computer games the most attractive. The possibility of using the spectroscopy teaching freeware available on the Internet is a remarkable help for teachers. The topics offered by our chemistry portal to students concern signal processing, spectra interpretation and the application of advanced chemometrics to spectroscopy. The course module on signal processing is presented in a separate publication, whereas the modules concerning spectra interpretation teaching and the application of some chosen chemometric methods in spectroscopy will be presented in this article.

## METHODS

Distance education through the Internet, making use of the state-of-art information and communication technologies is now an integral part of the "educational space". It makes possible not only permanent access to educational materials that are updated and put on WWW pages or FTP servers at any time or place but it also allows an interactive nature of teaching, access to discussion groups, chats and e-mail messaging. The developed IT tools also offer a few ways to support the person conducting the teaching process, they help to evaluate a student's activity, determine the extent of the material the student has already become familiar with, etc. The spectroscopy course we worked out is based on the Moodle educational platform. Its purpose is to help with teaching the basics of various spectral methods and the application of chemometric methods to spectroscopy when the instruction process is carried out by the traditional method, with the teacher and the pupil in the same classroom. The platform we used is freeware; it does not need sophisticated tools. Thanks to this it may be uploaded into most frequently used web servers, in any operational environment. While modifying and completing it with new solutions and tools, the creators of the Moodle software consider the feedback from its users. The latter discuss their problems and ideas how to improve the platform with the creators of the project on discussion forums on the official website of the project.

The blended learning course that has been developed teaches have to approach issues concerning signal processing, molecular spectra interpretation and application of advanced chemometrics in spectroscopy. Thus, the multimedial lessons (e-lessons) of the course available on the [www.e-chemia.pl](http://www.e-chemia.pl) portal are used to enhance the teaching of the three above mentioned skills. The syllabus provides students with the information about e-lessons for self-teaching and their final execution date and also gives information about which lessons will be run in the traditional way in the classroom and when. The knowledge and skills that students will acquire as a result of the e-lessons are indispensable to discuss and resolve the problems given by the teacher in the classroom. For example, 30% of the course on spectra interpretation is done by the student alone with the use of e-lessons available on the portal. The lessons sequentially teach the student a) spectra-structure correlations, i.e. relationships between structural features of chemical compounds and their characteristic spectral features in IR, UV-Vis, <sup>13</sup>C NMR, <sup>1</sup>H NMR and MS spectra, b) the application of the correlations he learnt to predict, for a given structural formula, which signals will arise in the real spectrum of the compound and c) determination of the structure of a compound from its spectrum. Class meetings are intended to solve more difficult problems whose solution requires the teacher's suggestions as the way of arriving at conclusions is difficult to present in a general procedure. Such a problem is the right combination of the structural information pieces obtained from individual types of spectra and then the creation of the structural formula of a chemical compound that is being identified.

The objective of e-lessons of the Advanced Chemometric in Spectroscopy is to prepare students to work with a real computer program which performs a selected chemometrics calculation on spectral data. The student is obliged to go through the e-lessons before a meeting with the teacher and performing real calculations in the computer laboratory.

The structure of the spectroscopy course is hierarchical (Fig.1). The course consists of three basic modules: Signal Processing Module, Spectra Interpretation Module and the Advanced Chemometrics in Spectroscopy Module. Each of these is divided into submodules concerning particular problems, e.g. kinds of spectral methods or kinds of chemometric methods: linear learning machine (LLM), linear discriminant analysis (LDA), k – nearest neighbour (k – NN), artificial neural networks (ANN), etc.. Consequently, the submodules are divided into lectures and laboratory exercises.

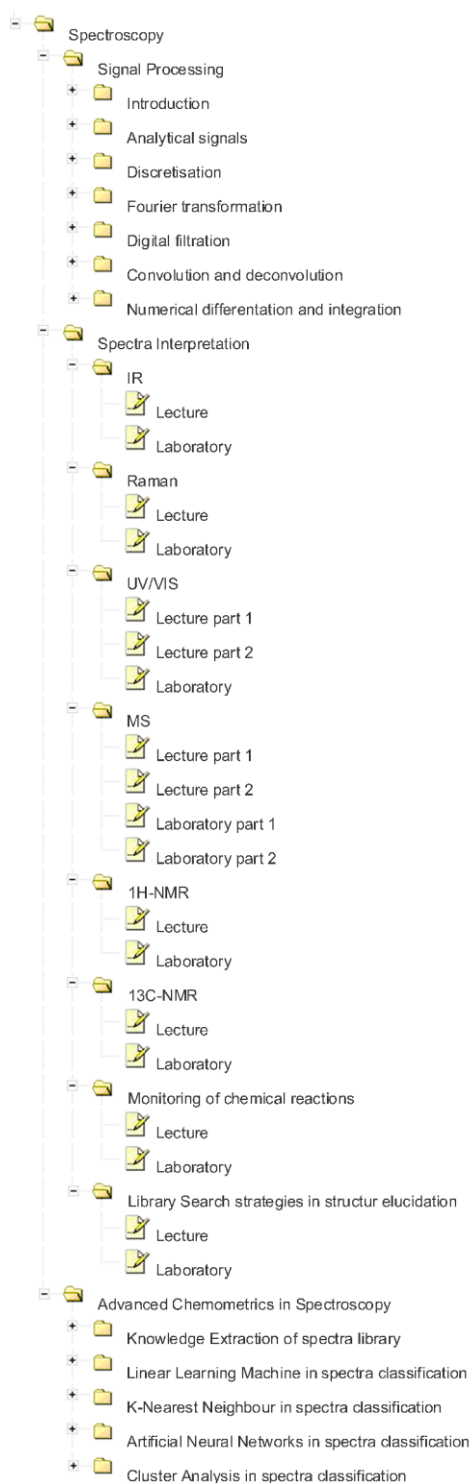


**Figure 1:** The structure of spectroscopy course.

The lab part of a given submodule consists of a few lessons whose parts are as follows:

- Introduction into the lesson - it gives the purpose of the exercise, the most important information necessary for carrying it out and practical indications in order to ease the completion of the task.
- Problems for a test - the part includes examples of test questions checking the student's knowledge of the problem being worked on which is necessary to conduct the exercise.
- Description of the exercise procedure - it gives all step-by-step activities to be conducted to properly complete the task, so, depending on a particular exercise:
- Examples illustrating the way how to carry out each exercise.
- Auxiliary materials for the lesson containing e.g. mathematical formulae or necessary numerical values.
- Tests checking the student's knowledge of the exercise done.

After the completion of these lessons contained in a given module the student has to fill up a test checking his knowledge acquired while doing individual exercises. The tests have a varied structure, among others there are test questions with multiple choice answers one of which is correct, multiple choice questions with many correct answers, questions with answers to be adjusted, questions involving filling in blank spaces. On the page with the question there appears feedback information about whether the answer was right or wrong, partial completion of the test, the final answer and the failure to give an answer.

The problems presented in the lecture part are illustrated with short films showing how the spectrometers work or the course of the processes occurring during the spectrum registration. In the laboratory part there are short instruction films teaching students how to do the calculations applying the specialist software, e.g. Statistica program offered by the StatSoft company (StatSoft, Inc. STATISTICA, 1998-2000).

Having familiarized with the problems related to the processing of signals registered by spectrometers (Signal Processing Module), the student learns how to use the spectra of a chemical compound for its identification by the method of traditional spectra interpretation (Spectra Interpretation Module). Then he is instructed how the process can be aided by chemometric methods (Advanced Chemometric in Spectroscopy Module).

## SPECTROSCOPY COURSE – SPECTRA INTERPRETATION MODULE

Spectroscopy is used for a wide variety of procedures in chemistry. However, at the simplest level it is routinely applied to identification of new molecules. Thus, our course "Spectroscopy" just serves teaching how to find out the structure of a compound based on its spectral features. At present the course is aimed at students who begin to learn how to use spectral methods to define the chemical structure of a molecule. The course teaches IR, Raman,  $^1\text{H}$ NMR,  $^{13}\text{C}$ NMR, UV-Vis and MS spectroscopies. The organization of the course is hierarchical: the division on spectroscopic techniques is higher, the kind of didactic lessons - lectures and laboratories is lower (Figure1).

Our course also includes the module "Chemical reaction monitoring" illustrating how to follow the progress of chemical reactions by spectral methods. The lecture part of the particular spectral methods discusses the theory of a given kind of spectroscopy and explains how spectrometers work by means of simulators. The laboratory part comprises problems concerning the correlation between spectra and structure in spectral methods- predicting the spectrum for a known structure and the interpretation of a spectrum, i.e. the recognition of the structure of a chemical compound based on an analysis of its characteristic spectral bands. In order to make it easier for students to understand more difficult problems, lectures and classes are

illustrated by animations. They show, e.g. molecular disintegration in a mass spectrometer, changing spectrum of the reagent as the chemical reaction continues, recording  $^1\text{H}$ NMR and  $^{13}\text{C}$ NMR spectra of a compound while the frequency is being "swept all over" or recording an MS spectrum with the changing intensity of the magnetic field.

Thus, the module of IR spectroscopy contains three lessons concerning organic compounds: a lesson teaching the student what bands are characteristic of individual function groups; a lesson on how to predict what bands to expect in the IR spectrum of a compound of a known structure and a lesson on how to recognize what structural fragments are present (or not) in a compound whose structure is not known. Teaching the spectral- structural correlations using a prepared lesson consists in watching bands characteristic of the selected function groups that are active in infrared. The bands are highlighted on the experimental IR spectra and the student has to know their description. The lesson comprises 14 units, each of which refers to one chosen class of organic compounds and contains a discussion on the characteristic spectral features of functional groups. It also gives standard, interpreted IR spectra with characteristic bands that are properly coloured and accompanied by the information about the related vibration. After becoming familiar with the description of the group frequencies, IR spectra and passing the test, the student is ready for doing the next exercise which consists in predicting bands characteristic of the given compound structure in IR spectrum. The purpose of the exercise is to prepare the student to face the situation when he, as a chemistry engineer, has to confirm the structure of a compound he already has some knowledge about, e.g. from the course of the chemical reaction. With help of correlation tables, the student can predict what bands should appear in the IR spectrum of a substance of a known structure. He defines the location of the bands, their intensity and shape. The student then checks the designed bands comparing them with the experimental spectrum he can find in the part of the lesson with answers, of the SCANKEE-MDS spectral database (Dębska & Guzowska\_Świder, 1999) or in the freeware Spectral Database for Organic Compounds in the Internet (SDBS, 2012). The way of designing IR spectra is illustrated in the lesson with an example involving a few compounds. There is also a commentary on the causes of possible differences between the designed and experimental bands. The lesson prepares the student to draw conclusions about the structure of a compound based on its IR spectrum. While doing the next lesson the student acquires the skill of recognizing the structural elements which can possibly make up a fragment of a molecule of the compound being identified as well as the ability to discard the fragments which cannot constitute a part of the molecule of the compound analysed. A few examples explain how to grade the unsaturation of the compound, assign structural fragments to the most intensive bands, confirm the presence of the recognized fragments based on their characteristic bands in other frequency areas and eliminate from consideration those structural fragments whose diagnostically strong bands do not occur in the spectrum analysed. The student learns to interpret IR spectra and decide which structural fragment and kind of vibration a particular band is related to. The student can also verify his conclusions as after the cursor has been positioned on the band, the information of its origin is displayed. After completing this task and doing the test well the student begins the lesson. He should have enough knowledge to independently interpret IR spectra of simple organic compounds in order to recognize structural fragments that are probably present in a molecule of the compound that is being identified.

The module also contains a lesson on how to correlate IR spectrum with the structure of inorganic compounds. The skill is exemplified with a few interpreted IR spectra with colour marked characteristic bands and information of what kind of vibration is related with IR spectrum. IR spectroscopy connected problems are also the subject of the lesson placed in the Raman spectroscopy module which is an

illustration of the complementary nature of the Raman and IR oscillatory spectroscopies. The objective of the lesson is to teach the student to practically use IR and Raman spectroscopies for the identification of organic compounds and explain how different choice rules of the two spectroscopies influence function group activity and spectrum picture. The Student, using the spectral-structural correlation tables and knowing the structure of the compound should be able to predict what typical oscillations will be performed by the individual structural elements of a molecule. Knowing that in IR spectroscopy oscillation is active if the dipole moment changes during vibration and that when oscillation causes polarization change then it can be observed in Raman spectrum the student tries to predict the possible differences and similarities between the IR and Raman spectra for the same substance. After that the student compares experimental IR and Raman spectra of the compound investigated and looks for bands stemming from the oscillation of the same structural element in the two spectra. It allows him to observe that a given oscillation of a structural element can be seen in either spectrum or only in one of them or produce bands of different intensity in both of them. The student, knowing the choice rules conditioning the oscillation activity in both IR and Raman spectroscopies, tries to explain the presence or lack of specific bands in the spectra investigated or different intensities of the bands. During the realization of the lesson of each module the student has easy access to the appropriate correlation tables without having to look for any outside source of information.

IR spectroscopy is also used in the module "Chemical reaction monitoring" which teaches how to apply spectral methods to verify a chemical reaction process, i.e. to check if the reaction runs as predicted and if the product obtained has the predicted structure. The method of checking the reaction process applied to these lab exercises consists in analysing the changes in IR (or  $^1\text{H}$ NMR) spectra of the substrate samples connected with the bands (signals) of reacting group. "Disappearance" of the bands that are characteristic of the substrate and "appearance" of those characteristic of the expected product evidence the assumed reaction course. Lack of the expected bands in the product spectrum suggests a reaction course different from the assumed one. Through interpretation of the spectra of the product obtained it is possible to determine its structure and formulate hypotheses regarding the actual course of the reaction. Relevant lab exercises have been prepared for the reactions students know from their organic chemistry course, whereas other advanced lab exercises are based on the records of the scientific research conducted at Rzeszów University of Technology.

The spectroscopy course in the [www.e-chemia.pl](http://www.e-chemia.pl) web portal is continually extended and not all planned modules are ready for use yet. However, lessons are being prepared now for all kinds of spectroscopy teaching how to predict spectra the same way that was described in the case of IR spectra. For UV-Vis spectra the lesson teaches to predict the band location of  $\pi$ - $\pi^*$  transfer for the given structure of an organic compound that belongs to dienes, enones or carbonyl derivatives of benzene based on the given Woodward-Fieser additivity rules and empirical parameters included in the lesson. However, for  $^1\text{H}$ NMR and  $^{13}\text{C}$ NMR spectra, the locations of the bands are determined based on the well-known additivity rules. In the case of  $^1\text{H}$ NMR spectra the student can predict the chemical shift values using the correlation tables and the designed spectrum is drawn with a spectrum creator, which allows the student to easily compare it with the experimental spectrum (Fig.2.).

For all kinds of spectral methods, tests are being prepared to check the student's knowledge of the application of spectroscopy to the identification of a chemical compound structure. Most test questions consist in associating the locations of spectral bands with the appropriate structural element (and vice versa) or matching the given structures with the right spectra.

## SPECTROSCOPY COURSE – ADVANCED CHEMOMETRICS IN SPECTROSCOPY MODULE

The lessons contained in this module teach to apply chosen supervised and unsupervised chemometric methods to analyse the data contained in spectral data bases in order to come to conclusions about the spectrum-structure interrelations.

### Supervised chemometric methods lessons

In the lesson Multispectral Database System students also learn to use spectral bases for the identification of chemical compounds by means of the library search method, i.e. comparing the experimental spectrum with spectra from the base in order to find spectra similar or identical with the spectrum of the compound that is being identified. The lesson uses the spectral base of IR, Raman, UV-vis, <sup>1</sup>HNMR, <sup>13</sup>CNMR and MS spectra of standard organic compounds students know from their organic chemistry course. The base stores spectra as spectral curves and values of locations and intensities of spectral bands as well as the coded structural formulae of their corresponding chemical compounds.

The module Multispectral Knowledge Formalizer illustrates how the application of statistical methods for the analysis of the spectral bands parameters enables automatic search (SCANKEE-MDS program, Dębska & Guzowska-Świder, 2012) for the relation between the structural fragment occurring in the molecule and the presence of a band (bands) in the spectrum. The program allows the student to perform automatic processing of the correlations into rules that form a knowledge rule base. The rules generated for the particular structural fragments and the observation of the bands in the spectrum of an unknown compound that is being identified allow finding out if the fragments can be part of the compound's molecule. The student can analyse the generated rules displaying them on a screen. Then, after uploading the spectral parameters of the bands of the identified compound into the program and starting up the reasoning module of the SCANKEE program, cooperating with the rule base of knowledge he can obtain a list of structural fragments that are probably present in a molecule of the investigated compound. In this way the student also gets to know the technology of building and generating expert systems as the automatically created knowledge rule base together with the concluding machine, makes up an advice expert system aiding the process of recognizing structural fragments constituting a molecule of the chemical compound under identification. In the lesson the automatic generation of spectral-structural correlation and then the knowledge rule base is exemplified by the base of spectra coded as 0/1 vectors where "1" means presence and "0" lack of a band in a given spectral range. The last component of the compound's vector includes a piece of coded information about the presence/absence of a given structural fragment in the compound's molecule.

The same base of molecular spectra vectors is used in the lessons illustrating the application of some supervised pattern recognition methods to classifying spectra into categories. The lessons show the student that the chemometric methods make it possible to carry out spectra classification in such a way that the spectra of a specific chemical compound comprising a definite functional group will form a cluster of points distant from the set of points representing the spectra of compounds without the group in multidimensional space. The student watching such sets of points is convinced that these techniques can be used for an automatic recognition of the structural features of substances based on their spectra.

The student makes himself acquainted with these techniques by first using linear learning machine for spectra classification and checking if the created decision vector properly defines the membership of the test set spectra. The student makes use of various model spectra sets, i.e. linearly separable ones and those that are not linearly separable. In case when the programme cannot create a decision vector (iteration process does not coincide) dividing a given spectra set into categories, the student discovers that the LLM method does not always lead to success, i.e. in this

case it does not help to identify the type of the compound. In this situation the student checks if another chemometric method, e.g. k-NN method enables solving the problem of compound identification. In this method one always gets a result because, assigning the object (spectra) to the appropriate category is based on assigning the object investigated (spectra) to the category that the nearest points belongs to. The student's task is to evaluate the correctness of this classification. The spectra classification by the LLM and k-NN method is conducted by the student with the SCANKEE-MLC (Dębska & Guzowska-Świder, 2003) program.

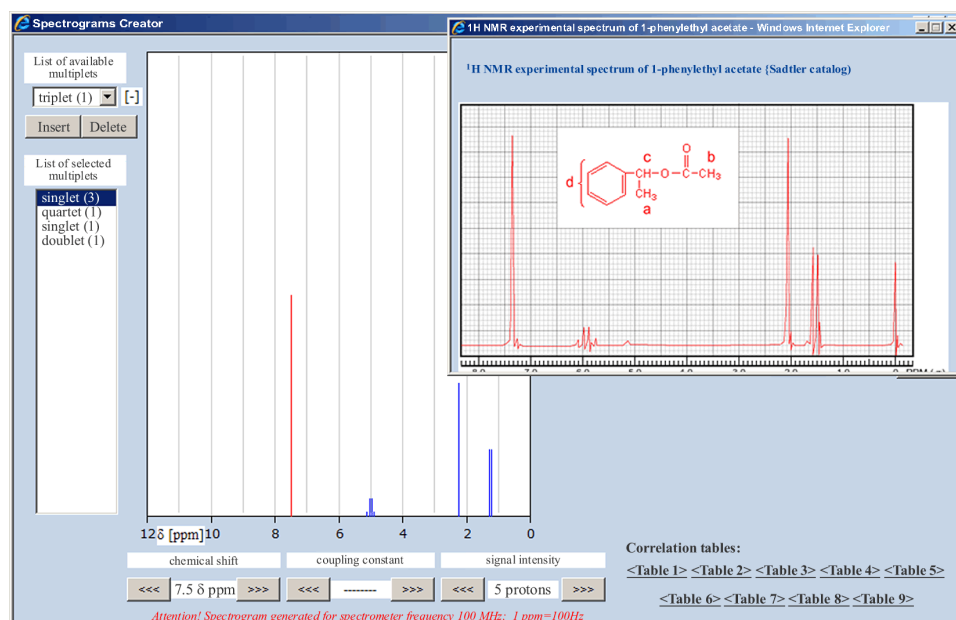


**Figure 2:** The student can compare the designed  $^1\text{H}$ NMR spectrum with the experimental one.

In order to get acquainted with the possibility of applying artificial neural networks to spectra classification the student, using still the same base of molecular spectra vectors, generates neural networks (Fig.3.) to recognize the type of compound using the Statistica Neural Networks PL version 4.0F program. At first the student uses the module of the Intelligent Problem Solver Program which automatically selects the optimum network architecture and teaching algorithms. During a successive lesson the student, having some previous experience, designs the networks and decides on how to teach it.

Conducting a sensitivity analysis the student can evaluate which spectral intervals are of crucial importance in the spectra classification process, i.e. are characteristic of a given type of the compound.

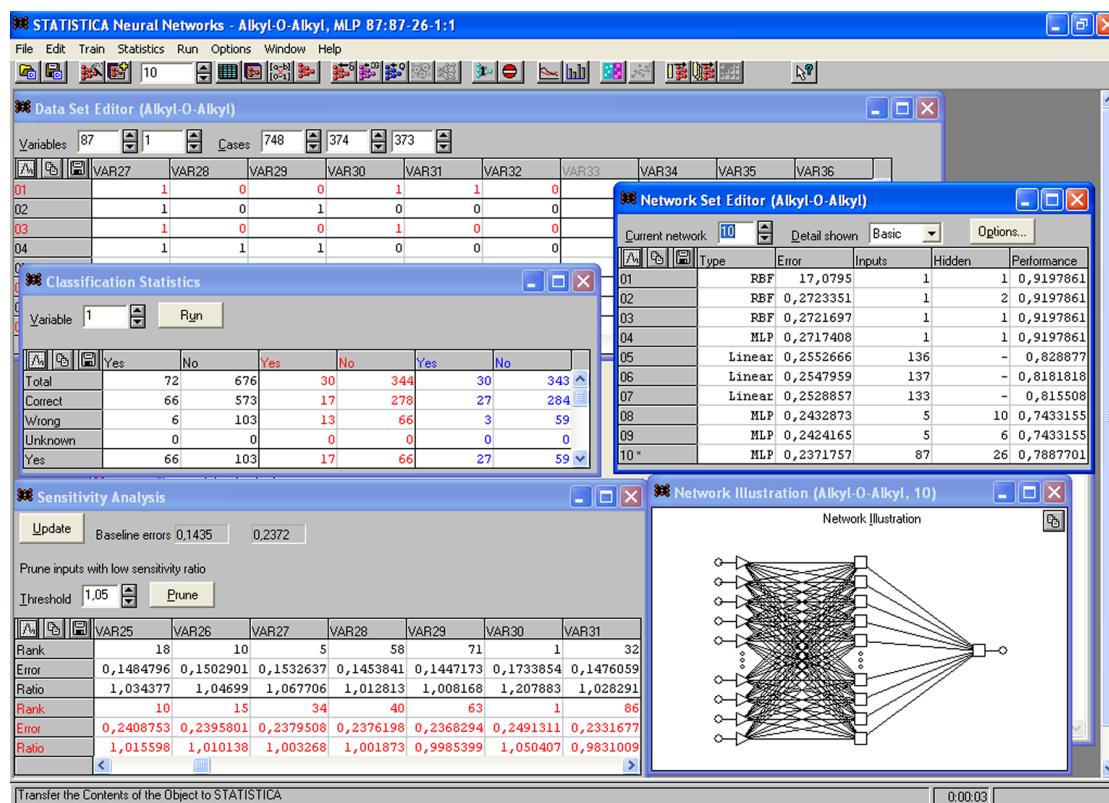
### Unsupervised chemometric methods lessons

The application of unsupervised chemometric methods to spectra classification is presented to the student on the example of cluster analysis carried out with VVT programme (Dębska & Wianowska, 2002). The lesson makes use of the base of spectra vectors that was applied in the lessons on supervised chemometric methods but modified by removing the information about to what specific kind of compound the spectrum belongs. The student generates decision trees for various spectra sets and evaluates, at different levels of similarity coefficient values, if the formed clusters belong to the same class of chemical compounds.

### Course evaluation

The elaborated spectroscopy course available through the [www.e-chemia.pl](http://www.e-chemia.pl) portal was evaluated according to the selected quality criteria developed by the Asso-

ciation of Academic E-learning in Poland (Association of Academic E-learning in Poland, n.d.). The word “selected” indicates that the AAE criteria are designed to assess a single online course with an exclusively distance education via the Internet. However, the selected criteria can be used as guidelines for the preparation and realization of the e-learning components of blended learning courses or courses face to face supported by e-learning.



At the end of the spectroscopy course, students filled out a questionnaire containing questions on the e-learning part of the course concerning its organization, development and realization with a particular emphasis on the didactic aspects of the course. Up to 95% of the students did not have any problems using the course, due to its e.g. availability at any time, even through the mobile, availability of plug-ins, easy navigation in the course, and easy operation of the software. About 90% of the students positively estimated the educational aspect of the course: its didactic means (simulations, interactive tasks, self-assessment test, etc.) and the content. Generally, the course seemed to them to be more user-friendly than the printed materials.

## CONCLUSION

The spectroscopy course that has been drawn up is used by our students as a didactic aid for subjects which deal with issues concerning signal processing or those requiring the skill of molecular spectra interpretation. The course is also of use in the case of subjects related to chemistry informatics where chemometric methods are taught.

Work on creating new modules of the [www.e-chemia.pl](http://www.e-chemia.pl) course and improving the already existing ones is ongoing. Successive spectrometer models illustrating the

principle of obtaining spectra are being made and relevant tests extended by adding new questions. Also, a module teaching how to identify the structure of an organic compound by interpreting a few kinds of its spectra registered with the use of different spectral techniques is being developed and new lessons on chemometric methods are being prepared.

The construction of the educational portal for students at the Chemistry Department of the Rzeszów University of Technology is fully justified by social and educational needs. It is also an implementation of the ministry recommendation (Law on Higher Education, the act passed on July 27th, 2007 which requires that part of university classes be conducted using methods and techniques of distance education) and in accordance with the priorities of the "European Union Policy. EU Human capital operational programme 2007-2013 priority IV. Tertiary education and science" concerns, among other things, preparation and implementation of didactic programs and materials in the e-learning form (Detailed description, 2009).

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