Pakistan Journal of Applied Sciences 1 (4): 516-521, 2001

Identification and Determination of Some Metals by Expert System

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Abstract: The recognizing of some metals, which have a significant role in the pollution of environment is the focus of attention in hygiene and environmental surveillance. These metals, mainly including copper, zinc, cobalt, lead, and nickel, usually pollute the environment even though to a little degree, and when they exceed a certain degree, they change into toxic pollutants. For this reason, they are referred to as toxic metals. The identification of these metals is carried out in other applications such as pharmacology, toxicology, and atmosphere pollutants. In analytic chemistry, the application of classical methods, due to low concentration, (the low cost methods and which need precise measurement instrument) is not applicable in a certain substance. As a result, it is necessary to use voltammetric methods. These methods are more exact and more expensive and they need more precise laboratory instruments. Since there are several methods (voltammetric methodology), tools (electrods) and environmental conditions for the test, and that working process must be properly directed by intermediate results of test and observation of the results by a chemical expert, the use of an expert system in this case can be extremely useful. This article introduces the implementation of an expert system for supporting the identification of trace metals with low concentration.

Keywords : Chemical Analysis, Expert system, Pollutants

Introduction

Experts are valuable resources for any organization. However, human experts are expensive, retired, and perishable. Therefore, if expert's knowledge to be computerized, It will be remained and support organization forever.

Expert systems are computer's software that is used for the purpose. one of the aspects of science, that expert systems may be applied, is chemical. A chemical expert system's target is computerizing of a chemical expert's knowledge and reasoning. For this purpose we are tried to develop an expert system for voltammetric analytics. This expert system is formed from three expert module. In this article, we briefly explain main expert system's concepts, then explore each of the module .

For several trace metal determination, versatile and powerful voltammetric procedures have been introduction in recent years. Although electroanalytical techniques are much cheaper than other techniques with similar detection limits, They are not very popular. Because of the existence of instrumentation which is reliable, sensitive and commercially available, at low cost, well tested routine methods for toxic metal determinations in environmental surveillance, food control, occupational medicine, toxicology and hygiene(Numberg, 1984) and a wide rang of potential users (with in sufficient electroanalytical foundations). The development of an expert system may be of great interest in order to guide the application of voltammetric methodologies. Such systems have already been applied in several branches of analytical chemistry, especially liquid chromatography (Vanleeuwen *et al.*, 1990), liquid, liquid extraction (Moors and Massart 1990), spectrophotometry (Janssen and Espen 1986 and Verbeke *et al* 1986) and AAS(Browett, 1989). In the electrochemical filed, also expert system for the elucidation of electrode reaction mechanisms has been reported (M. Palys *et al.* 1990 and 1991).

The Expert System: There are two major trains of an expert that to be modeled in system. The expert's knowledge and reasoning. To accomplish this the system must have to principal modules. A knowledge base and an influence engine. The knowledge base contains highly specialized knowledge on the problem area as provided by the expert. It includes problem facts, rules, concepts and relationships.

The inference engine is the knowledge processor which is modeled after the expert's reasoning. The engine works with available information on a given problem, coupled with the knowledge stored in knowledge base , to draw conclusion or recommendations . In this article , the out aim is design of a knowledge base for the problem.

Expert System for Voltametric Methods: The our expert system is made up of three expert modules which are activated in a hierarchical order. In this activation, the first module checks only some conditions of the sample and if the sample has proper conditions for the voltammetric test, then the determination activity is passed onto the second and the third modules. The second and the third modules, in turn, support the chemical expert in recognition of presence of the metals in the sample. Generally speaking, Figure 1 shows architecture of knowledge base and the function of each of the modules.

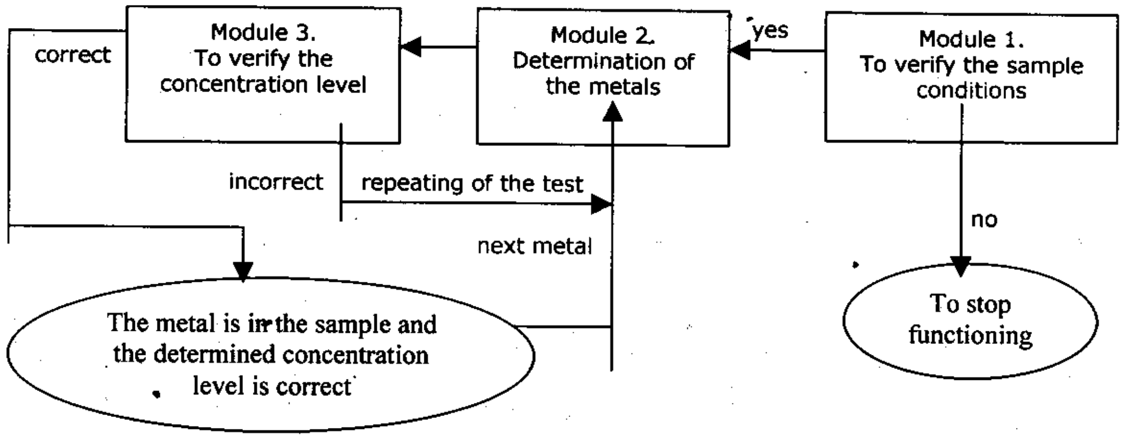

Fig.1: Architecture of the knowledge base for PMI

Module 1. Exploring of optimal condition for the sample treatment. that to be tested.

Module 2. Based on the domain expert-proposed concentration level and the analysis of results, this module directs the test and verifies the presence of the metals.

Module 3. This module verifies the correct domain expert-proposed concentration level for each of the metals, and if it is not correct for some metals, the module recommends a concentration level and the repetition of the test.

First Module, The Analysis of the Conditions of the Sample: The purpose of this module is to verify the proper conditions of the sample for the test. Fig. 2 illustrates the inference network for the first module. The knowledge base of this module which consists of the following 17 rules analyzes sample substance and the testing environment.

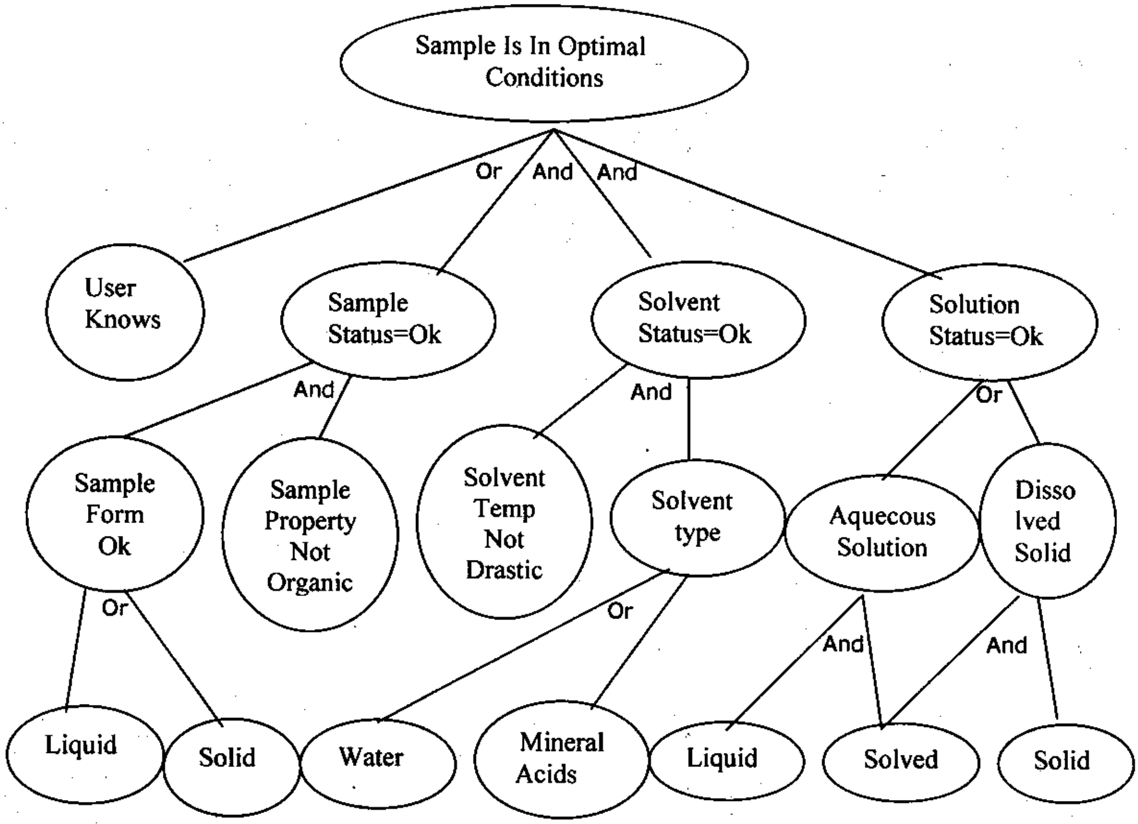

Fig. 2: Inference Network for Module 1

Primitives:
Sample Form : solid / liquid / unknown / gaseous
Sample Property: with organic / not organic / unknown
Solvent Temp: high / normal / unknown
Solvent Type: water / mineral acid / others
Sample Solved: solved / not solved / not completely solved / unknown

- If the domain expert knows that sample conditions are favorable, the next module is performed (sample testing).
- If the domain expert knows that the sample condition is not favorable, then this sample can not be analyzed and the system stops functioning.
- If the domain expert does not know the sample conditions, PMI tries to determine sample status by posing questions to the domain expert. Moreover, PMI itself , verifies environment conditions too (solvent and dissolved). The three proper conditions include:

- the sample must be in favorable conditions;
- the solvent of the sample must be in favorable conditions;
- the dissolved sample must be in favorable conditions;

The favorable conditions for the sample:
- It should be either solid or liquid;
- No gaseous or unknown form can be tested;
- It should not include organic substance;

The favorable conditions for solvent:
- No high temperature, the domain expert determines high or normal temperature;
- It should be either water or mineral acids;

The favorable conditions for solution (dissolved sample)
- Aqueous or dissolved solid;
- The aqueous solution is one that is obtained by thorough solving of a liquid sample in a solvent .
- The dissolved solid is one that is obtained by thorough solving of a solid sample in a solvent.
- If the sample can not solve in a solvent, or it is almost solved, or the dissolving is not known, the solution is not favorable.

Second Module, The determination of Trace Metals: This module is activated, when the sample enjoys the favorable environmental conditions. The module covers the following three purposes:
- To recommend a proper method and to direct that method for sample testing, and to analyze the metals in question.
- Regarding the domain expert observations, the verification of at least a single peak in sketched curve of the test.
- To select one or more metals by domain expert for their recognition in the sample substance And then to interact between domain expert and PMI to verify the observed peaks and corresponding them to the metals.
- The use of a voltammetric method for the determination of trace metals depends on the selected concentration level. This level maybe quite different for different type sof metals. The level limits for each of the metals is recorded in the form of facts in knowledge base. If there are too many metals, a database can be used.

The expert system specifies the following three cases:
- The metal concentration in the sample is less than the lowest specified level. Therefore, if the method does not show the metal in the sample, the metal is either absent or it has so low concentration level that the voltammetric method can not determine it. In this case, because of very low concentration, the presence of this metal is not so significant.
- The metal concentration in the sample is more than highest specified level. In this case, the presence of the metal in the sample is definite, but the voltammetric method is expensive and not suitable; therefore, the classic method is recommended.
- The metal concentration in the sample is in one of the three specified concentration levels. In this case, the proper corresponding voltammetric method is recommended by the expert system.

Procedure in Module 2: At first, the domain expert is required to guess one of the three concentration levels. This concentration level is taken for each of the five metals and then a proper corresponding method for the selected one is recommended by the expert system. Based on this recommendation, the domain expert carried out the test. When the method is applied, the domain expert proclaims his observations obtained from the resultant curves to the expert system. If the selected metals concentrations are different (which is the case in most instances), the expert system reports each of the found metals to the domain expert. If there is no trace of any metals, the either the metal is unavailable or the proposed method has not been suitable. If this is the case, a proportional method to the metal concentration should be recommend, so that the domain expert applies another voltammetric method for the metals not found in the sample. Then domain expert reports his observations to the expert system. Table 1 shows level limits for each metal and corresponding voltammetric method for the test. If the concentration level, guessed by the domain expert, is unknown, above the first level, or below the third level, no method is recommended or selected. Consequently the expert system stops functioning.

Table 1: Level Limits for each metal and corresponding method

Concentration Level	Method	Level
$1.0 \times 10^{-5} < Ni < 1.0 \times 10^{-3}$	Pol	1
$1.0 \times 10^{-5} < Co < 5.0 \times 10^{-3}$	DME	
$1.0 \times 10^{-5} < Cu < 5.0 \times 10^{-5}$		
$1.0 \times 10^{-5} < Zn < 1.0 \times 10^{-3}$		
$5.0 \times 10^{-5} < Pb < 1.0 \times 10^{-3}$		
$1.0 \times 10^{-6} < Ni < 1.0 \times 10^{-5}$	taste-Pol	2
$0.8 \times 10^{-6} < Co < 1.0 \times 10^{-5}$	SMDE	
$8.0 \times 10^{-6} < Cu < 1.0 \times 10^{-5}$		
$1.0 \times 10^{-6} < Zn < 1.0 \times 10^{-5}$		
$1.0 \times 10^{-6} < Pb < 5.0 \times 10^{-5}$		
$1.0 \times 10^{-8} < Ni < 1.0 \times 10^{-6}$	DPP	3
$1.0 \times 10^{-8} < Co < 0.8 \times 10^{-6}$	HMDE	
$6.0 \times 10^{-8} < Cu < 8.0 \times 10^{-6}$		
$5.0 \times 10^{-7} < Zn < 1.0 \times 10^{-6}$		
$5.0 \times 10^{-8} < Pb < 1.0 \times 10^{-6}$		

The choice of the technique is mainly determined by the concentration of the analyte . In this system, usual techniques in trace and ultratrace analysis, such as differential pulse anodic stripping voltammetry(DPASV), differential pulse polarography (DPP), and differential pulse chatodic stripping voltammetry have been considered. The choice of the electrode is related to the concentration level and using techniques. Thus dropping mercury electrode (DME) , static mercury drop electrode (SMDE) and hanging mercury drop electrode (HMDE) have used.

In all cases, after the recording of the voltammograms, the expert system repeat the information needed to identify the peaks and to detect the presence of anomalous features by means of the values of the peak widths at half – height.

For each of the metals, specified by domain expert, to be analyzed by the expert system, the presence of corresponding peak in the resultant curve is After applying a voltammetric method, a voltammogram curve is sketched in the specified device. Fig. 3 shows a sample curve, obtained at Kashan University Chemical Lab. This sample includes several peaks. Each peak is represented by an arrow. These peaks, appeared in the curve, may indicate the presence of metals in the sample. Therefore, they must be further analyzed. This analysis is performed by asking the domain expert some related questions. After we ascertain the presence of peaks in the curves, the domain expert is required to determine the desired peaks. The specified metals are put on a stack, to pose questions regarding the presence of a peak for each of them in the curve. For each peak in the curve, if there is one, there is a correspondence voltage on the Y axis. If one peak voltages is not the same as the standard peak voltage of the metal, the metal is not available in the sample.

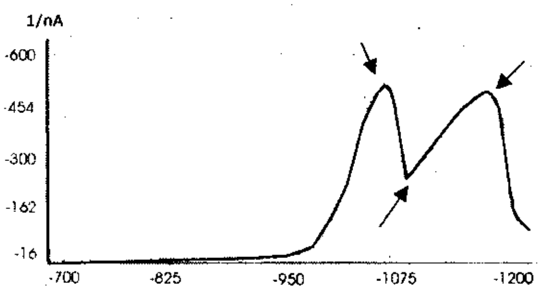

Fig. 3: A Voltammogarm curve that was obtained by a test

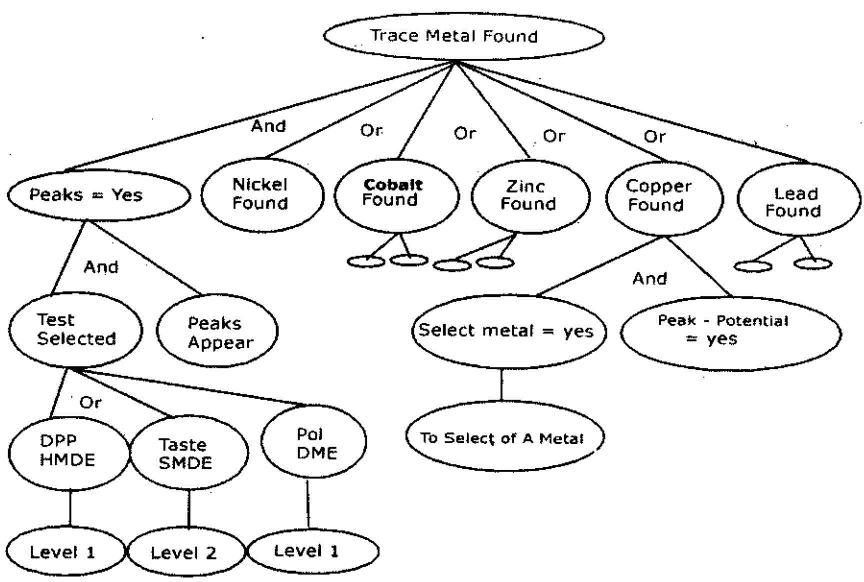

Fig. 4: Inference network for Module 2

Primitives:
Level : to select a concentration level
To Select A Metal : to select a metal
Peak Appears: observation of appearing of peaks
Peak Potential: voltage of peak th corresponding with a metal

Each metal, found in the sample, is put in a stack for further analysis so that in the next phase the degree of correctness of the selected concentration level by domain expert is determined. If the selected one is not correct, the expert system recommends one proper concentration level. Although the selected concentration level by the domain expert may result in the presence of the metal , the selected one can be determined more precisely. Fig. 4 shows the inference network for module 2.

Module 3, The Determination of the Correctness Concentration Level: For each of the metals for which a proportional peak in curve was found, the expert system asks the domain expert to sketch standard calibration line for the metal and to map the correspondence peak to the line. Fig. 5 shows a sample mapping.

In this module, the domain expert is asked:

- In which place of the smetal calibration line is the produced mapping located?

- To answer this question, the domain expert can select one of the three choices: over the calibration line, on the calibration line; or under the calibration line. In this case, the expert system recommends the following :

- If the produced mapping value is located on the calibration line, then the metal, with the specified concentration level, is present in the sample and the applied voltammetric method is proper. Consequently, the selected concentration level is correct for the metal.

- If the produced mapping value is over the calibration line, then the metal is present in the sample, but the applied concentration level is not proper, i.e., it can not be used to determine the metal concentration level.

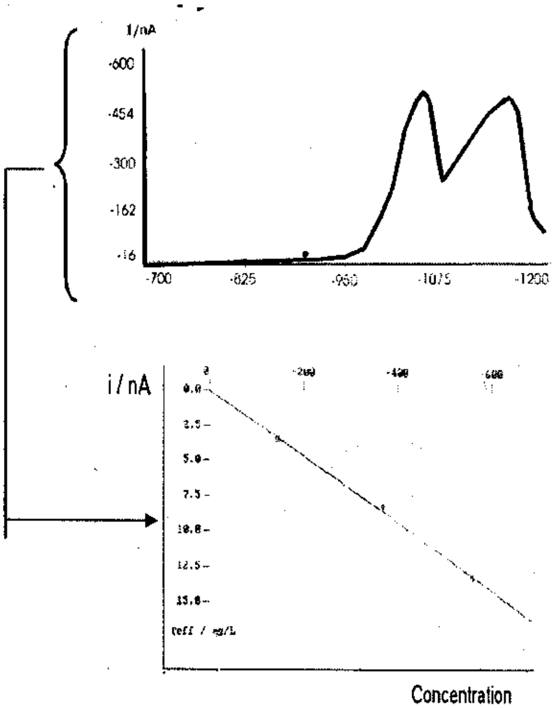

Fig. 5: Voltammogram curve and mapping of the upper peak to calibration line

- If the produced mapping value is under the calibration line, it is not clear whether or not the metal is present in the sample so further analysis is required.
- If the third level has been determined, the metal is not available in the sample.

If the second or first level has been determined, the lower concentration level must be selected. So the correct method should be determined and the test should be repeated. In the repeated test, the domain expert selects another concentration level, considering above-mentioned. If the metals have remained unknown in previous testing, or if no proper recognition method has been used, the domain expert further analyzes the metal. Fig. 6 shows inference network for module 3.

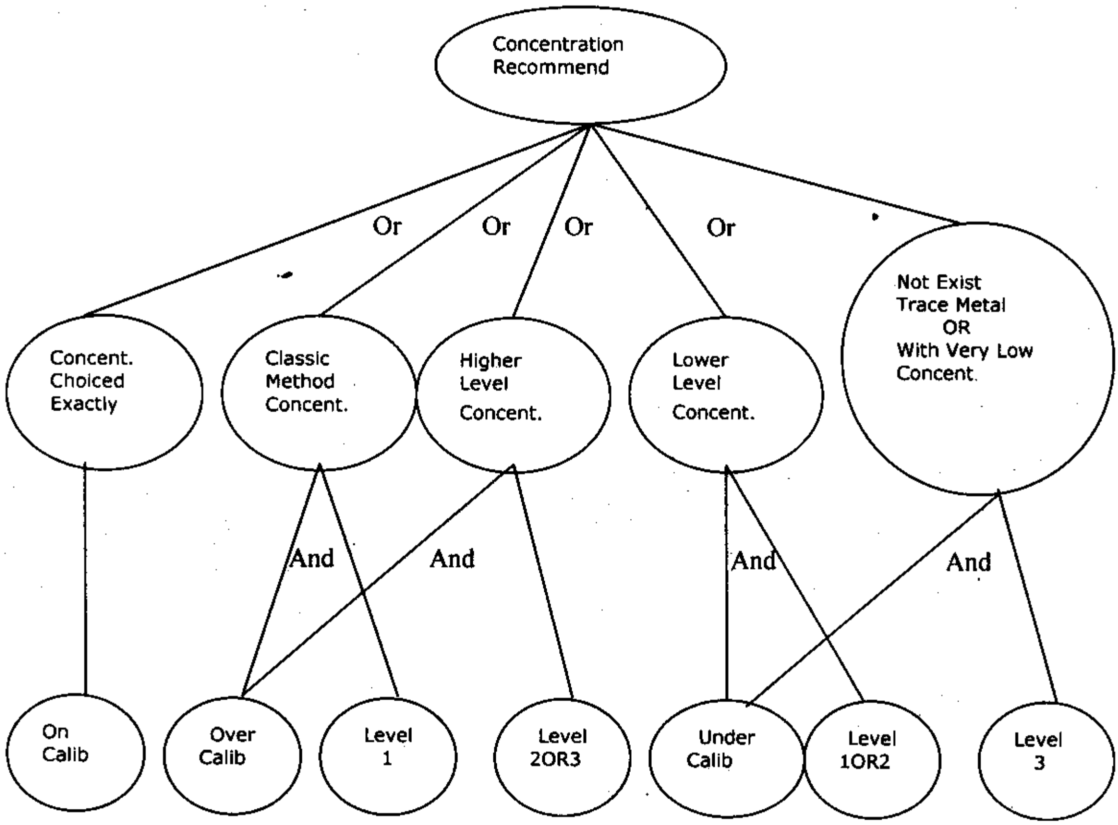

Fig. 6: Inference Network for Module 3

Primitives:

On Calib: the mapping of the peak is on the standard calibration line of the metal

Over Calib: the mapping of the peak is over the standard calibration line of the metal

Under Calib: the mapping of the peak is under the standard calibration line of the metal

Level : level of selected concentration

Conclusion

In this article, an expert system, was introduced for designing and implementation of pollutant metals identification. In practice, the implementation was carried out and the results were observed.

The results proved that this expert system is of considerable assistance to the domain expert in the testing path, and the domain expert was quite satisfied with the assistance. It is obvious that the domain expert is an intelligent user. Therefore, he can use the expert system more efficiently. This Expert system is more convenient with this type of users.

References

A. P. Wade, S.R.Crouch and D.Betteridge, 1988. Treands Anal. Chem.7, 358.

H. W. Numberg, 1984. Sci. Total Envion, 37, 9: Pure Apple. Chem., 54 (1982) 253; Anal. Chim. Acta, 164, 1.

J. Wang, B.Tian and J. lu, Talanta, 1992. 39, 1273.

J. Smeyers-Verbeke, M.R.Detaevernier and D. L. Massart, 1986. Ana. Chim. Acta, 191, 181.

J. A. Vanleeuwen, B.G. M.Vandeginste, G.Kateman, M. Mulholland and A. Cleland, 1990. Anal. Chim. Acta ,228, 145.

K. Janssen and P.Van Espen, 1986. Anal. Cheim. Acta, 191, 169 Anal. Chim. Acta, 191(1986) 181.

M. Moors and D.L. Massart, 1990. Trends Anal. Chem. 9, 164.

M. Palys, M. Bos and W.E.vander Linden, 1990. Anal. Chim. Acta., 231, 59; 248 (1991) 429.

R. E. Dessy, 1984. Anal. Chem. 56. 1200A, 1312A.

W. R. Browett, T.A.Cox and M.J.Stillman, 1989. B.A. Hohne and T.H. Pierce(Eds), Expert Systems Application in Chemistry, Acs Symposium Series, Vol. 408, Washington, P. 210.