IOSUD –„DUNAREA DE JOS" UNIVERSITY OF GALATI

Doctoral School of Mechanical and Industrial Engineering

PhD THESIS

SUMMARY

EXPERT SYSTEM FOR THE RECOGNITION OF CLASS IDENTITY OF HALLUCINOGENIC AMPHETAMINS

PhD student,

Cătălin NEGOIȚĂ

Scientific leader,

Prof. univ. dr. fiz. Mirela PRAISLER

Series I4: Industrial Engineering Nr. 72

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	Conf. dr. fiz. Steluța GOSAV, "Dunarea de Jos" University of Galati

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GALAȚI

2020

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Foreword

At the end of this important period of study and research, I would like to thank to all those who have contributed to my trening, encouraged and supported me throughout these years.

I would like to thank Prof. Dr. Mirela Praisler, my scientific coordinator, for the effort and patience she showed, as well as for all the guidance I received, which helped me enormously to complete this scientific work.

Many thanks to Prof. Dr. Luminița Moraru, Assoc. Prof. Dr. Steluţa Gosav and Prof. Dr. Habil. Constantin Apetrei from the “Dunărea de Jos” University of Galați, members of my Guidance Commission, both for the support provided and the suggestions offered during the doctoral study.

Galați, September 2020 Fiz. Cătălin Negoiță

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Introduction

In the current context of modern society in economic and social terms, there is a continuing challenge in fighting all forms of organized crime, as modern society has come to be greatly influenced by it. The high-risk drug market occupies a large segment of the organized crime activity worldwide. We can consider that the challenge in terms of drug detection exists in all its phases, whether we are talking about their synthesis, design, production, distribution networks or consumption.

Drug trafficking poses a serious threat to public safety and health, both nationally and globally. Globalization, along with the rapid development of technology, the diversification of trade links, the creation of new routes and methods of transport, and the elimination of border controls, lead to the development of criminal organizations fueling and controlling the illicit drug market. Unfortunately, Romania is also included in this international network. Cases when Romanian citizens have been involved by criminal groups as international carriers have been reported. In recent years, increasing attempts to import synthetic drugs of abuse (amphetamines, methamphetamines, amphetamine derivatives, etc.) from countries with a tradition in producing synthetic drugs (Belgium, the Netherlands, Germany) have been noticed. Such transports have been detected through maritime, air or land transportation routes [1].

Unfortunately, modern technology also comes to the aid of these structures, leading to a slight advantage in their favor. Modern methods of production and smuggling are applied in order to avoid controls from law enforcement. This highlights the need to develop new modern analytical techniques able to detect quickly and efficiently the controlled compounds, especially the substances with psychotropic effect.

Very often, the clandestine laboratories try to circumvent the law by slightly changing the molecular structures of the compounds that are already listed as controlled substances. They are adding or changing one or more substituents present in the molecular structure of the parent drug of abuse, hence obtaining a substance that is not listed as controlled substance, but still preserves the pharmacological activity of the parent compound, or a very similar one.

Since the instruments currently used in customs, airports, ports, etc., can efficiently identify only those drugs of abuse that are known and included in the controlled substance lists, the legislators and law enforcement institutions encourage the development of more efficient analytical instruments, which are able to detect any new compound having *a* **molecular structure that is similar, and not only identical,** to the known drugs of abuse.

Such and objective may be reached by combining spectroscopic techniques with modern class identity assignment techniques that can be developed by using artificial intelligence models.

Artificial intelligence applications are developed in an increasingly larger variety of fields, such as industry, medicine, political and social sciences. **The results presented in this thesis point out that the proposed combination of spectroscopic and artificial intelligence methods is appropriate for developing successful toxicological and forensic applications. The expert systems that have been developed and presented in this thesis are a contribution to the development of the industrial engineering, as they may operate control instruments that are currently industrially produced.**

Abstract and thesis structure

This doctoral thesis, entitled "Expert system for the class identity recognition of hallucinogenic amphetamines", is structured in four chapters that are accompanied by an introduction. The final section presents the general conclusions that were drawn based on the original contributions, as well as the future directions of research and development.

This paper begins with an introduction, which underlines the need for new techniques able to detect and identify banned substances that are produced, transported and marketed by illicit drug trafficking networks or organized crime.

Chapter I describes the general properties of the targeted hallucinogenic amphetamines, as well as the list of the compounds chosen for analysis in this thesis.

Chapter II contains the presentation of the main spectral methods are used for the characterization and identification of hallucinogenic amphetamines. The chapter describes the basic concepts of infrared spectrometry, the basic components of a spectrometer and elements of the theory associated with these techniques.

Chapter III, entitled "Methods of artificial intelligence applicable to the recognition of the class identity of organic substances", describes the six artificial intelligence techniques that have been used for building the expert systems, i.e. PLSR, Genetic Algorithms, KNN, Random Forest, SVM and Logistic Regressions. This chapter presents an overview of these algorithms, the functions and methods of interpretation, as well as the theoretical considerations necessary for evaluating the performance of the expert systems based on the evaluation of errors and confidence intervals.

Chapter IV, entitled "Contributions on artificial intelligence applications designed to recognize the class identity of the main 2C-x and DOx hallucinogenic amphetamines", presents the original contributions to the development of the expert systems that have been build, based on the methods theoretically presented in Chapter III, and which are designed to screen for the 2C-x and DOx hallucinogenic amphetamines described in Chapter I.

The section dedicated to the general conclusions presents a final comparative analysis of the performances of the artificial intelligence methods. The synthesis of the results points out the most efficient expert system that should be used for the detection of the targeted hallucinogenic amphetamines. **This is the system that is recommended for**

implementation at industrial engineering level, i.e. in the mass production of the portable instruments used by law enforcement.

The thesis ends with a short description of the personal contributions presented in this thesis, as well as with the list of papers that have been published and / or presented at national and international conferences.

Motivation of choosing the research theme

In recent years, artificial intelligence has been increasingly used in almost all fields. The improvement of the performances regarding the screening based on FTIR and ATR-FTIR spectra is of major importance. The models presented in this thesis can be successfully used to other fields, such as medicine engineering, chemical engineering, etc.

The use and purchase of high-risk drugs is a growing danger to modern society and the effort of all institutions in the fight against trafficking networks can be supplemented by the development of expert systems such as those based on models presented in this doctoral thesis. Besides its efficiency, such systems have another very important advantage: they can be used to operate portable analytical instruments that can be used in field operations for *in situ* screening.

These two aspects may have a great impact on the future of modern society. Digitization and automated screening systems based on artificial intelligence methods may be important assets for the fight against organized crime networks. The performances of the six studied models indicate that they have a high potential to increase the performance of class identity recognition of hallucinogenic amphetamines.

Pursued research objectives

The following research objectives have been pursued in this doctoral thesis: literature research regarding the current state of the art, identification of the compounds of interest and of the most appropriate spectral methods used for the characterization and identification of targeted hallucinogenic amphetamines, choice of the artificial intelligence methods having a high potential of generating efficient expert systems designed to operate analytical instruments used for the detection of the targeted drugs of abuse.

As a result of the theoretical analysis of the models proposed for study and research, the following objectives have been pursued in the phase of the model development:

- building the data base with the spectra of the compounds of interest;
- identification of the parameters of each studied model that could lead to the optimization of the model and the implicit improvement of the classification performance;
- evaluation of the performances of the expert systems built with each of the considered artificial intelligence techniques, by comparing the results obtained for the complete

data base and a data set selected by using the genetic algorithm and which contains only the most relevant information;

- running the models in several iterations with varied and fine-tuned parameters;
- comparative analysis of the performances of the expert systems built with these techniques, for two data bases, in order to identify the best performing system.

LIST OF PUBLICATIONS

ISI publications

- **Indexed in the Thomson Reuters Web of Knowledge – Web of Science (WoS) database**

1. **Negoita, C.**, Praisler M., Ion, A., Artificial Intelligence Application Designed to Screen for New Psychoactive Drugs Based on their ATR-FTIR spectra, *Proceedings of the 10th Jubilee International Conference of the Balkan Physical Union BPU10*, 26-30 August 2018, Sofia, Bulgaria. Mishonov, T. M., Varonov, A.M. (Eds), *AIP Conference Proceedings*, vol. 2075, issue 1, Article number 170026 (2019). DOI: 10.1063/1.5091391 **WOS:000472653800274**
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