IOSUD –"DUNAREA DE JOS" UNIVERSITY OF GALATI

Doctoral School of Mechanical and Industrial Engineering

PhD THESIS

ABSTRACT

INTELLIGENT SYSTEM FOR AUTOMATIC DETECTION OF HALLUCINOGENIC AMPHETAMINES

PhD. student,

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Scientific Coordinator,

Prof. univ. dr. fiz. Mirela PRAISLER

Series I 4: Industrial Engineering No. 71

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Keywords: NBOMe hallucinogens, Artificial neural networks (ANN), Molecular descriptors, DFT, ATR-FTIR.

Introduction

The term of "drug" has several meanings, with no single definition. Thus, in order to define this concept, several criteria are needed, such as: psycho-activity (ability of the substance to influence the human psychic), medical utility (substances that are intended to cure different diseases of the human body), illegality (substances whose possession / marketing are illegal) or the public definition (substances called by the civil society as drugs, for example coffee). Drugs can be defined as psychoactive substances whose production, marketing or unauthorized possession (for other purposes than medical or scientific purposes) is prohibited.

Overdose is a multipurpose problem among drug users. Drug-related morbidity and mortality associated with somatic causes, such as HIV / AIDS, hepatitis and liver failure, acute renal and respiratory failure, suicide and violence, have increased in recent years [1]. According to data presented in the 2019 World Drug Report, prepared by the United Nations Office on Drugs and Crime (UNODC), nearly 271 million people aged 15-64 have consumed at least once, more precisely 5.5% of the global population. This study indicates that one in 18 people use drugs and that there is an alarming increase in drug use worldwide, with almost 30% between 2009-2017 [2].

The drug market is in continuous development, the drug traffickers using modern technology for their production and innovative methods for smuggling, in order to circumvent controls and seizures. Drug trafficking can be characterized in two ways: amateur trafficking (which uses relatively small quantities, usually for personal consumption) and international trafficking (targeting large quantities and carried out by professionals who are part of illicit or even terrorist organizations).

Trafficker networks permanently synthesize new compounds, by slightly modifying the molecular structure of the basic illicit substances, more precisely by adding / changing some substituents from different positions of the basic molecular structure, which are meant to generate substances that are not yet found on the list of controlled substances, but which largely preserve the psychotropic properties of the initial substances. Because these newly designed substances are not yet on the list of controlled or prohibited substances, law enforcement authorities cannot take measures to criminalize drug traffickers before updating the official list.

On the other hand, the process of identifying and characterizing new chemical structures by toxicologists requires precious time and substantial analysis costs. As such, the development of computer applications that allow the significant acceleration of this analytical process is essential. Moreover, traffickers are known to use advanced drug hiding techniques. These applications can be used for the rapid *in situ* detection of controlled substances and even remote monitoring (wiring) of clandestine laboratories where drug production and / or storage takes place.

Illicit drug trafficking remains one of the most serious threats to public health and safety, both globally and nationally. There are not to be neglected nor the activities of money laundering from drug trafficking, which often serve to finance illegal activities, for example those of a criminal nature or correlated with international terrorism.

Drug trade is an extremely profitable source of financial resources and can generate instability in both the countries of origin and the countries in transit. To combat drug trafficking and terrorism worldwide, various intergovernmental and governmental organizations have been set up in this regard, such as: International Drug Control Board-International Narcotics Control Board (INCB), International Criminal Police Organization (Interpol)), The United Nations Office on Drugs and Crime - Narcotics Commission, World Customs Organization, International Financial Action Group (FATF), etc. [3-8].

The summary and structure of the scientific work

This PhD thesis is entitled „Intelligent system for automatic detection of hallucinogenic amphetamines" and was organized in 5 chapters, accompanied by a brief introduction, general conclusions and future directions of study.

The introduction presents a description of the evolution of drug use worldwide, as well as how the population is affected globally, by the fact that trafficker networks permanently synthesize new compounds with extremely high toxicity, which can cause death, which are sold. on the black market for their stimulating and hallucinogenic effects.

Chapter I describes the main hallucinogenic substances of abuse, as well as new hallucinogenic compounds, which have been discovered after the 2000s. The latter compounds have a high toxicity. Overdoses representing lethal intakes have been reported worldwide.

Chapter II presents the ATR-FTIR spectral methods that have been used for the characterization and the identification of the studied hallucinogenic amphetamines.

Chapter III, entitled „DFT method combined with chemometric methods applied to recognize the class identity of hallucinogenic amphetamines", describes the DFT method and models of artificial neural networks (Artificial Neural Networks, ANN) used in the thesis for building automatic systems designed to detect the hallucinogenic amphetamines of interest.

Chapters IV and V present the author's personal scientific contributions regarding the development of intelligent systems built for the automatic detection of hallucinogenic amphetamines, respectively the artificial intelligence applications that have been developed for the automatic recognition of the class identity of the main hallucinogenic amphetamines and especially of one of the most recently discovered classes on the black market, the NBOMe hallucinogenic amphetamines.

Chapter IV presents the applications that have been developed for the recognition the class identity of the compounds of interest based on their ATR-FTIR spectra and in Chapter V those developed on the basis of their molecular descriptors.

General conclusions summarize the performances and limits of the intelligent systems of automatic detection of the developed hallucinogenic amphetamines and the main original results obtained during the doctoral thesis.

The thesis ends with a description and the motivation of the main future directions of study. Finally, the list of scientific published in prestigious scientific journals papers, as well as of those communicated at national and international scientific conferences, is presented.

Motivation for choosing the research topic

Synthetic drugs have experienced significant worldwide expansion in recent years. During the last decades, there has been a significant increase in drug use, especially among adolescents and young adults. New synthetic derivatives, with effects similar to hallucinogenic drugs but not yet under legal control, are sold on the illicit market as drugs such as LSD or MDMA. Among these new substances are hallucinogenic compounds with high toxicity, which can cause death.

The use of narcotic substances is a phenomenon that has grown and is directly proportional to the number of deaths recorded globally. Most research suggests that adolescence is a critical period of risk for initiating illicit substance use. The period of initiation among adolescents of drug use is today between the ages of 12-14 years, up to 15-17 years. Adolescents who use drugs up to the age of 18-25, are likely to struggle with addiction later in life and have permanent and irreversible brain damages.

Another major problem is that these drugs can be purchased online through illicit channels, and their consumption is quite high. Drug use among high school students is a major problem. Both their parents and teachers need to be sufficiently well informed about illicit substances and especially of the effects of the use of these substances, in order to identify adolescents with problems, their good information on the effects of drug use and providing support to prevent relapse.

The negative effects of drug use include: emotional problems (anxiety, depression, suicidal thoughts, schizophrenia), behavior problems (aggression, theft), addiction, health problems (HIV / AIDS, hepatitis B and C), learning problems (short or long term memory impairment), brain damage (permanent brain deterioration, such as brain contraction; impaired learning skills; impaired reasoning, perception and intuition, and severe impairment of the nervous system), as well as accidents (especially cars).

As a teacher, I think that the safety of the citizen, the prevention of antisocial facts, as well as the education of the young generation in the spirit of the law, are priorities for civil society, especially in the area and the area adjacent to the school units.

Pursued research objectives

The main scientific objectives of the thesis referred to:

- Carrying out a literature research on the current state of art regarding:
  - Hallucinogenic amphetamines, especially NBOMe compounds;
  - ATR-FTIR spectra;
  - Applicable chemometric methods for recognizing the class identity of hallucinogenic amphetamines, especially ANN networks;
- Carrying out scientific research in the following directions:
  - Vibrational analysis of new hallucinogenic amphetamines based on ATR-FTIR spectra;
  - Optimization of the molecular structure of the new hallucinogenic amphetamines;
  - Computational study of 3,4-methylenedioxypyrovalerone;
  - DFT characterization of the MDMA methylene homologue, a chemical compound with psychoactive properties;
  - Physico-chemical characterization of new hallucinogenic amphetamines based on molecular descriptors;
  - Artificial neural networks designed to identify NBOMe hallucinogens using molecular descriptors.

These studies are necessary because the database formed with new substances designed in clandestine laboratories must be constantly updated so that the law enforcement authorities can criminally hold those who produce, hold, market and / or illegally consume illicit substances. From the point of view of the process of identification and detection of the new chemical structures by the toxicologists, we should mention that this process is costly and long lasting. For this reason, world, European and national authorities in the field encourage the researchers to develop analytical solutions that allow the identification of new illicit substances as quickly and efficiently as possible. This thesis describes such solutions, developed on the basis of spectroscopic and artificial intelligence methods, with applications in industrial engineering, pharmaceutical industry and medical engineering.

Notations and abbreviations

UNODC	The United Nations Office on Drugs and Crime / Biroul Națiunilor Unite pentru Droguri și Crime
INCB	International Narcotics Control Board / Comitetul Internațional de Control al Stupefiantelor
INTERPOL	The International Police Organization / Organizația Poliției Internaționale
ONU	Organization of United Nations / Organizația Națiunilor Unite
WCO	Worlds Customs Organization / Organizaţia Mondială a Vămilor
FATF	Financial Action Task Force / Grupul de Acţiune Financiară Internaţională
LSD	Lysergic acid diethylamide / Dietilamida acidului lisergic
MDMA	3,4-Methylenedioxymethamphetamine / 3,4-Metilendioximetamfetamina
IUPAC	International Union of Pure and Applied Chemistry / Uniunea Internațională de Chimie Pură și Aplicată
SNC	Nervous central system / Sistem Nervos Central
DEA	Drug Enforcement Administration / Agenția de combatere a drogurilor din Statele Unite
MDA	3,4-methylenedioxyamphetamine / 3,4-metilendioxiamfetamina
MDPV	3,4-Metilenedioxypyrovalerone / 3,4-metilendioxipirovalerona
5-MAPB	1-(benzofuran-5-yl)-N-methylpropan-2-amine/ 5-(2-metilaminopropil)benzofuran
MDAI	5,6-methylenedioxy-2-aminoindane / 5,6-metilendioxi-2-aminoindan
7-APB	7-(2-Aminopropyl)Benzofuran / 7-(2Aminopropil) Benzofuran
PMEA	N-ethyl-4-Methoxyamphetamine / N-Etil-p-metoxi-alfa-metilfeniletilamina
NBOMe	N-methoxybenzyl-methoxyphenylethylamine / N-metoxibenzil-metoxifeniletilamina
2C-I	2,5-dimethoxy-4- phenethylamine iodine / 2,5-dimetoxi-4-iodofeniletilamina
25I-NBOMe	4-iodo-2,5- dimethoxy-N-(2-methoxybenzyl)phenethylamine / 4-iodo-2,5-dimetoxi-N-(2-metoxibenzil) feniletilamina
25H-NBOMe	2-(2,5-Dimethoxyphenyl)-N-[(2-methoxyphenyl)methyl]ethanamine / 2-(2,5-Dimetoxifenil)-N- [(2-metoxifenil) metil] etilamina
25C-NBOMe	2-(4-Chloro-2,5-dimethoxyphenyl)-N-[(2-methoxyphenyl)methyl]ethan-1-amine / 2- (4-cloro-2,5-dimetoxifenil) -N - [(2-metoxifenil) metil] etil-1-amină
NBOMe-TCB-2	N-[(3-bromo-2,5-dimethoxy-bicyclo[4,2,0]octa-1,3,5-trien-7-yl)methyl]-1-(2-methoxyphenyl)methanamine / N - [(3-bromo-2,5-dimetoxi-biciclo [4,2,0] octa-1,3,5-trien-7-il) metil] -1- (2-metoxifenil) metilamina /
Cimbi-31	2-(8-Bromo-2,3,6,7-tetrahydrofuro[2,3-f][1]benzofuran-4-yl)-N-(2-methoxybenzyl)ethanamin / 2-(8-bromo-2,3,6,7-tetrahidrofuro [2,3-f] [1] benzofuran-4-il)-N-[(2-metoxifenil) metil] etilamina /
25B-NBOMe	N-(2-methoxybenzyl)-2,5-dimethoxy-4-bromophenethylamine / N-(2-metoxibenzil)-2,5-dimetoxi-4-bromofeniletilamina

25TFM-NBOMe	2-(4-trifluoromethyl-2,5-dimethoxyphenyl)-N-[(2 methoxyphenyl)methyl]ethanamine / 2-(4-trifluormetil-2,5-dimetoxifenil)-N-[(2-metoxifenil) metil] etilamina
25D-NBOMe	2-(2,5-dimethoxy-4-methylphenyl)-N-(2-methoxybenzyl)ethanamine / 2-(2,5-dimetoxi-4-metilfenil)-N-(2-metoxibenzil) etilamina
25G-NBOMe	2-(2,5-dimethoxy-3,4-dimethylphenyl)-N-[(2-methoxyphenyl)methyl] ethanamine / 2-(2,5-dimetoxi-3,4-dimetilfenil)-N-[(2-metoxifenil) metil] etilamina
25E-NBOMe	2-(4-ethyl-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine / 2-(4-etil-2,5-dimetoxifenil)-N-(2-metoxibenzil) etilamina
25P-NBOMe	2-(4-propyl-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine / 2-(4-propil-2,5-dimetoxifenil)-N-(2-metoxibenzil) etilamina
25iP-NBOMe	2-(2,5-Dimethoxy-4-propan-2-ylphenyl)-N-[(2-methoxyphenyl)methyl] ethanamine / 2-(2,5-dimetoxi-4-propan-2-ilfenil)-N-[(2-metoxifenil) metil] etilamina
25N-NBOMe	2-(2,5-Dimethoxy-4-nitrophenyl)-N-(2-methoxybenzyl)ethanamine / 2-(2,5-dimetoxi-4-nitrofenil)-N-(2-metoxibenzil) etilamina
25T4-NBOMe	2-[2,5-Dimethoxy-4-(propan-2-ylsulfanyl)phenyl]-N-(2-methoxybenzyl) ethan-1-amine / 2-[2,5-dimetoxi-4-(propan-2-ilsulfanil) fenil]-N-(2-metoxibenzil) etil-1-amină
25T7-NBOMe	2-[2,5-Dimethoxy-4-(propylsulfanyl)phenyl]-N-[(2 methoxyphenyl) methyl] ethan-1-amine / 2-(2,5-dimetoxi-4-propilsulfanilfenil)-N-[(2-metoxifenil) metil] etil-1-amină
UV	Ultraviolet / Ultraviolet
VIS	Visible / Vizibil
IR	Infrared / Infraroșu
FTIR	Fourier Transform Infrared / Transformata Fourier în infraroșu
ATR	Attenuated Total Reflection / Reflexia totală atenuată
DFT	Density Functional Theory / Teoria funcționalei de densitate
B3LYP	Becke, 3-parameter, Lee–Yang–Parr / Funcționala hibridă cu 3 parametri a lui Becke care utilizează funcționala de corelație LYP formulată de Lee, Yang și Par
LDA	Local Density Approximation / Aproximația densității locale
GGA	Generalized Gradient Approximation / Aproximația generalizată a gradientului
ANN	Artificial Neural Network / Rețea neuronală artificială
BP-ANN	Artificial Neural Network with Back Propagation algorithm / Reţea neuronală multistrat cu retropropagare
NSE	Normalized Standard Error / Eroarea standard normalizată
R^2	Coefficient of determination / Coeficientul de determinare
MSE	Mean Square Error / Eroarea pătratică medie
RMSE	Root Mean Square Error / Rădăcina pătrată a erorii pătratice medie
MAE	Mean Absolute Error / Eroarea medie absolută

MPE	Mean Percent Error / Eroarea procentului mediu
RSE	Relative Squared Error / Eroare pătrată relativă
TPR	True Positive Rate / Rata de adevărate pozitive
TNR	True Negative Rate / Rata de adevărate negative
FPR	False Positive Rate / Rata de false pozitive
FNR	False Negative Rate / Rata de false negative
CR	Classification Rate / Rata de clasificare
CCR	Correct Classification Rate / Rata de clasificare corectă
ACC	Accuracy / Acuratețea
E	Error / Eroarea
MEP	Molecular electrostatic potential diagram / Diagrama potențialului electrostatic molecular
PED	Potential energy distribution / Distribuția de energie potențială
E_{HOMO}	Highest Occupied Molecular Orbital energy / Energia celui mai înalt orbital molecular ocupat
E_{LUMO}	Lowest Unoccupied Molecular Orbital energy / Energia celui mai jos orbital molecular neocupat
DM	Dipol Moment / Momentul de dipol
MM+	Molecular Mechanics + / Mecanica moleculară +
AM1	Austin Model 1 / Modelul Austin 1
PM3	Parametrization Model 3 / Model de parametrizare 3
QSAR	Quantitative Structure–Activity Relationship / Relația cantitativă structură-activitate
QSPR	Quantitative Structure–Properties Relationship / Relația cantitativă structură-proprietăți
SWGDRUG	Scientific Working Group for the Analysis of Seized Drugs / Grupul științific de lucru pentru analiza substanțelor medicamentoase confiscate

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