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An Overview Computational Intelligence Solution in Forensic Drug Analysis

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***Abstract*: In the past decade, computational intelligence has been widely applied in various fields to performing the task that are difficult or expensive in cost using conventional techniques. CI aims to ease the burden of human on a specific task. It is widely applied in various fields such as electrical engineering, computer science, business, and electronic and communication engineering. Hence, this has successfully drawn the attention from the researchers. The purpose of this paper is to present the application of CI in forensic drug analysis. In this paper, we present an overview of the CI techniques in various molecular structure research. We will study how CI techniques including genetic algorithm, artificial neural network, fuzzy logic, and hybrids of these techniques, could be employed to study the variety of different molecular structures such as protein, gene expression, and DNA structure. In addition, this application review also aims to present a concise survey of articles appearing in publication that appeal to forensic drug analysis. A brief explanation of several forensic drug analysis techniques that employed in the industries laboratory has been provided. Besides, several key articles have been selected to describe how CI techniques have been practiced in the forensic drug analysis within the scope of each of the discipline areas.**

***Keywords*:** Forensic Drug Analysis, Molecular Structures, Computational Intelligence, Artificial Intelligence

I. Introduction

Over the past decade, there are broad increasing in the illicit manufacturing of new and unfamiliar synthetic drugs that release to the market. The producers continuously invent new drugs by altering the chemical composition of the drugs substances and distribute illegally to generate huge profits. Although there are many illicit drugs can be used for medical purpose (treating a disease or a symptom), but consumption of illegal drugs without the assistance of medical professionals can lead to drug abuse. Drug abuse can also be known as drug addiction is a phenomenon where people become dependent to the drugs and they will start craving for it. Most of the drug abuse is targeting the human's brain, central nervous system (CNS), which will cause high impart to the human body due to the seizure of the illegal drug substance. Drug abuse has become a major problem that faced by the law enforcement official today, and identification of drugs and the compounds that make up the drugs is the main concern by the forensic chemist's job. Forensic chemist's will undergoes a series of processes performed in the laboratory in order to analyze and identify the presence or absence of controlled substance in the drugs that submitted by the law enforcement. Basically, drug of abuse (DOA) testing consists of two main types of laboratory testing process used in various drug analyses: Preliminary analysis and Confirmatory analysis. It is a two tiered process, which the laboratory must conduct preliminary analysis tests followed by a confirmatory analysis test to confirm the result from the preliminary analysis test. Preliminary analysis, also known as presumptive test is a test that presumed the absence or presence of drug substance based on the nature of the substances without further information. It is based on physical examination or observation, such as color, smell and taste of the physical powder, capsules, liquid and etc. Furthermore, PH (acidity, alkalinity) and specific gravity can also take into consideration. However, confirmatory analysis provides a further investigation follow by the presumptive test. Normally, confirmatory analysis is required when the presumptive test result is positive; to confirm the substance's identity. Hence, it is clear that presumptive test is less precise as compare to confirmatory test. Confirmatory tests are more accurate and specific in determining the type of substances present in the drug specimen using the instrumental analysis [1]. However, the experimental studies of confirmatory tests for drug identification involved multi-step process and expensive due to its high cost of R&D and time-consuming. An overview of the chemical analysis process of controlled substances that consists of many steps are shown in Figure 1.

Therefore, to overcome this drawback, numerous developments in informatics and computer science offer new opportunities. Generally, the principle of forensic drug chemistry in the illegal drug identification follows the chemistry discipline, which examine how the molecule in the drugs are bonded to each other. Hence, there are numerous researches that apply computational intelligence techniques for the molecular identification in the biomedical area. In order to present the literature review, the well-established and most representative work is classified into three main categories of computational intelligence techniques, which is Genetic Algorithm, Artificial Neural Network, and Fuzzy Logic. In addition, we also discuss and review some

representative methods that used in laboratory for forensic drug analysis and how CI techniques have been applied in the process to provide an ease of the burden of forensic chemist.

The rest of the paper is organized as follows: in Section 2, an overview of the computational intelligence methods that successfully applied in the complex molecular structure is supplied. Section 3, provides a brief explanation of various techniques that used in laboratory forensic drug analysis process and highlights the role of various computational intelligence approaches in forensic drug analysis. Section 4, concludes this paper by sharing the main insights in this research.

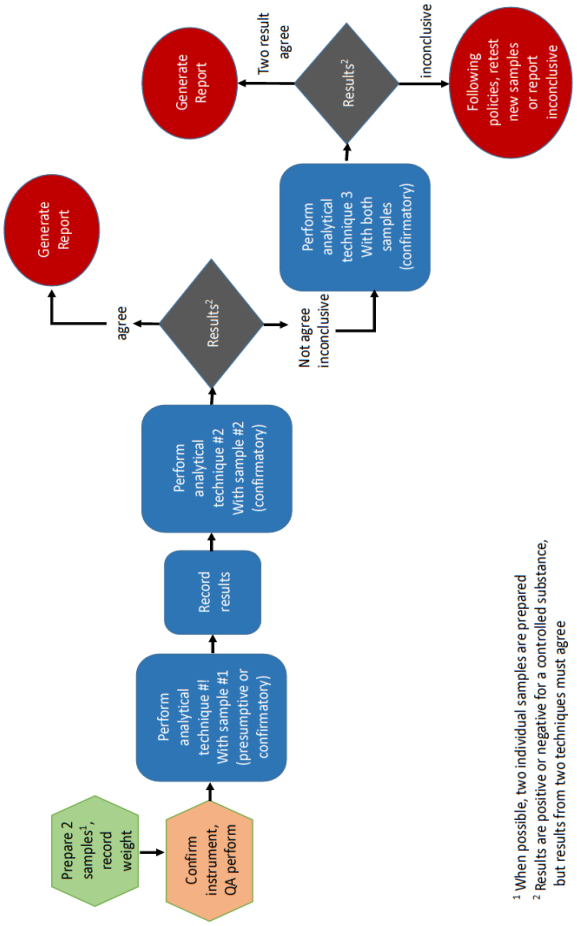

Fig. 1. An overview of the chemical analysis process of controlled substances [25].

II. Overview of Computational Intelligence Techniques

In this section, a comprehensive review of the employed computational intelligence techniques will be given, which including Genetic Algorithm, Artificial Neural Network, and Fuzzy Logic. In addition, a brief discussion of hybrid techniques is presented. In the Section 3, it will be reviewed how these techniques are implemented in the forensic drug analysis process.

A. Genetic Algorithm (GA)

Genetic algorithm (GA) is heuristic search that proposed by John Holland in 1975. It is a heuristic search technique that used to solve optimization problem for the problem at hand. The basic concept of GA is based on the Charles Darwin, the theory of evolution, the principle of "survival of the fittest" in the natural biological evolution in The Origin of Species [2]. GA is used to search the best population by following the basic step in Figure 2. Initially, a population is generated randomly. Next, a fitness function is applied to evaluate the fitness of each individual in the population. The fitness score will be passed to the breeding function to produce new and better parent population through selection, crossover and mutation process. This cyclical process will be repeated until a convergence criterion is met.

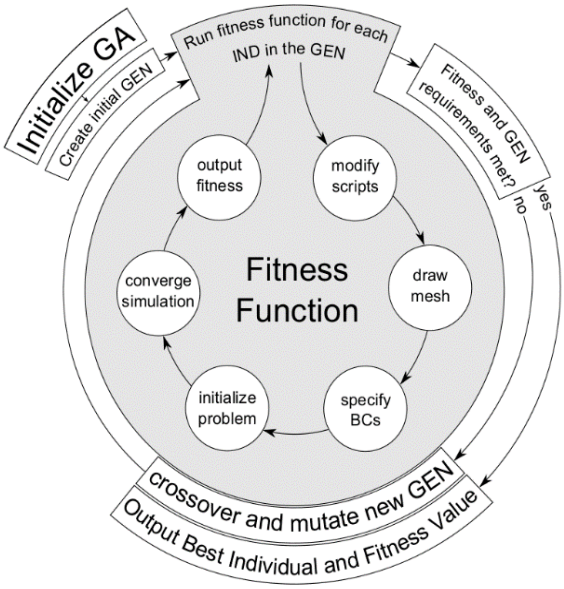

Figure 2. Flow chart of the cycle of the genetic algorithm.

David Fogel et. al. pointed out that there are several advantages of using evolutionary computation such as genetic algorithm techniques over traditional techniques. The advantages include conceptual simplicity, broad applicability, better performance than classic methods on real problems, potential to use knowledge and hybridize with other methods, parallelism, robustness to dynamic changes, capability for self-optimization, and the ability to solve problems that have no known solutions.

J. Solomon, et al. [4], applied genetic algorithm in parameterization of interatomic potentials for Metal oxides. In this study, they proved that genetic algorithm based methodology are capable to reproduce and energize the structure, capture the basic structural, mechanical, and thermal properties of the BTO (a member of an important class of metal oxide) and predict the two crystalline phases of the BTO.

P. Wałejko, et al. [5], developed a system using genetic algorithm (GA) to perform structural analysis of Phenyl galactopyranosides using C MAS NMR spectroscopy and conformational analysis. Conformational analysis was performed using genetic algorithm-assisted grid search

method (GAAGS), which is a technique that using search technique and genetic algorithm approach to increase the conformational analysis performance.

Z. Li, et al. [6], used the genetic algorithm with the multi-population evolution and entropy-based searching technique with narrowing down space to solve the optimization model for molecular docking problem. This proposed approach has evaluated based on RMSD value and it has achieved a rate of 41% excellent docking solutions, 38% of good docking solutions and 13% of poor docking solutions.

T. Paul and H. Iba [7] developed Probabilistic Model Building Genetic Algorithm (PMBGA) for the identification of informative genes for molecular classification and present the unbiased experimental results on three benchmark data sets. According to [8] genetic algorithm provides a better percentage of accuracy in identifying patterns between HIV-1 protease against organic leads and FDA approved inhibitors of HIV-1 protease.

Mahmood et. al [] introduced a graded and hybrid energy function with genetic algorithm (GA) to develop an ab inito PSP tool. The authors employed an enhanced genetic algorithm (GA) framework for protein structure optimization on 3D face centered-cube (FCC) lattice model. With the FCC lattice model, the maximum degree of freedom and the high resolution folding within the lattice constraint can be achieve and prediction with FCC lattice model can yield the densest protein core. Additionally, the FCC orientation will then align a real protein into the closest conformation amongst the available lattice configurations.

(Jeong et al. 2015) explore the used of Non-dominated Sorting Genetic Algorithm II (NSGA-II) to identify the appropriate e DNA locations for species-specific primer design. Athough the problem space for this research is small compared to other MOO analysis result, but the result show that the proposed method successfully searched for the consecutive locations with high potentialitybeing specific primer. Importantly, this study with the applicability of f NSGA-II to genomic DNA will help to discover the specialized locations from unknown, very complex groups of genomic DNA sequences.

B. *Artificial Neural Networks (ANN)*

ANN is inspired by biological neural network of the structure and functional aspect of the human being nervous system especially the human's brain [9]. ANN are popular today because it works by simulating the human intuition in decision making and can tolerate with complex, noisy and incomplete data. They are useful to learn complex relationships or patterns hidden in large scale dataset.

C. Lorenz, et al. [10] used artificial neural network to successfully identify mosquito species based on the molecular mosquito DNA samples. It is proved that the ANN has better classification performance than traditional discriminant analysis with high accuracy ranging from 85.70% to 100%.

According to Y. Li, et al. [11], it is proven that the artificial neural network model has a high performance in identifying complex, multi-dimensional and non-linear patterns than response surface methodology in the optimization of controlled release nanoparticle formulation of verapamil hydrochloride.

W. Laosiritaworn, et al. [12], proved that the ANN has a successful performance in modeling spin-transition behavior in ultra-thinfilm molecular magnet. In [13], the artificial neural network has been applied to predict the solubility of sulfur dioxide in different ionic liquids. The study proved that ANN can be a new alternative approach to predict different thermodynamic properties (solubility in this case) of the materials with the lowest error rate about 2%.

A. Ghaedi, et al. [14], applied artificial neural network to predict the density, viscosity, thermal expansion coefficient, molar volume and viscosity deviation of ethylene gly-col monoethyl ether (EGMEE) solution. In his study, he reveals that the ANN model can be an excellent alternative for simultaneous prediction of the thermodynamic properties of the aqueous solution of EGMEE with mean square error (MSE b 0.0051%) and high coefficient of determination (R2≥0.9913).

C. *Fuzzy Logic*

Fuzzy logic concept was first introduced by Zadesh in 1965 [15]. It provides mathematical tool for dealing with linguistic variables to describe the relationship between the system variables. The membership function in fuzzy logic can range within the interval [0-1]. Hence, fuzzy logic is suitable to apply in many fields due to its specialty in dealing with uncertainty and complexities data. The Figure 3 shows the membership function of temperature, i.e. low, medium and high.

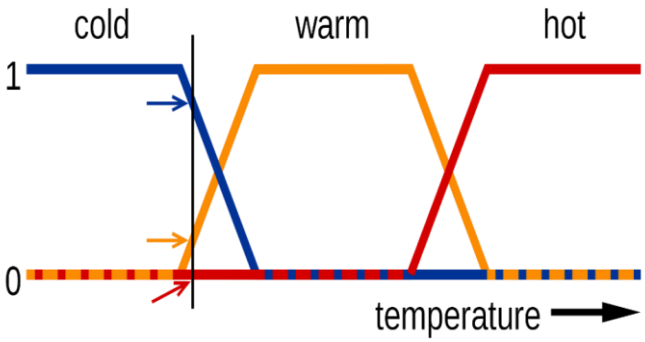

Figure 3. Fuzzy logic representation of temperature [24].

Saravanan and Lakshmi [16], applied a novel fuzzy rule based system for assessing the protein for allergenicity and evaluate the quality of the query protein. This system is helpful in distinguishing the allergen-like non-allergens from allergens and providing a uniform examination and interpretation of the results.

Sun, et al. [17], applied the dynamic fuzzy modelling approach for modelling genetic regulatory networks from gene expression data. This approach is useful in utilized the structural knowledge of gene network and the nonlinear dynamic property embedded in the gene network can be well collected. Hence, this approach can achieve a faster convergence in the identification process and the fuzzy gene network will have a better performance in prediction.

C. Umoja, et. al. [18] used the fuzzy logic and shape definition approaches to reduce the search size and predict the

possible molecular docking location. In [20], it has applied a fuzzy-logic based system for both diagnosis and control of a convention process of ammonia into nitrogen gas by different microbial groups. In addition, the fuzzy logic control module was tested and evaluated using dynamic simulations and has shown to achieve high and stable nitrogen removal efficiency (around 90%).

(Murilo et al. 2010) applied fuzzy cognitive models in molecular distillation process. The main benefit of the fuzzy cognitive models the use of an input/output data set together with qualitative information. Hence, the authors had feed the model with the distillation temperature and the feed flow rate as the input variables, and they take few parameter to measure the output responses, such as liquid interface temperature, the film thickness, the concentration profiles, and the distillate flow rate.

D. Hybrid Techniques

In a lot of others cases, a combination of different techniques is better than any single one.

K. A. Theofilatos [19], has successfully combined genetic algorithms with Extended Kalman Filters, and applied the combination for protein interaction prediction and classification. This combination is proven to be useful and effective if the search parameter is big and complex or it does not have a valid mathematical analysis of the problem.

M.E. Hamzehie and H. Najibi [21] used artificial neural network and Deshmukh-Mather model to predict the solubility of carbon dioxide (CO2) in amino acid salt solutions. Besides, in a hybrid approach, (Deng et al. 2016), applied an artificial nearon network based on genetic algorithm to predict the boiling point of refrigerants from 16 molecular groups and a topological index. The proposed model evaluated by the Deng et. al. showed a better performance with experimental data as compared with the develop numerical model and the other two existing models, namely QSPR approach and UNIFAC group contribution method.

In [22], the electron conformational–genetic algorithm (EC-GA) method is presented as a novel hybrid 4D-QSAR approach for pharmacophore identification and bioactivity prediction using the best subset of parameters. Besides, it also stated that the genetic algorithm manages to show the importance of thermodynamic, electronic and geometric parameters.

III. Forensic Drug Analysis

In this section, it is shown how the computational intelligence approach of Section 2 is used in the field of forensic drug analysis. Forensic drug analysis represents a number of disciplines that aimed to assist in the detection and interpretation of drugs for medico-legal purposes. These analyses can be carried out with the blood, urine and hair samples. The forensic drug chemists will be analyzing the given samples of unknown substances (powder, capsules, liquid, stain and etc.) to identify the presents of the chemical substances that make up the samples. Suspected illegal drug can be evaluated qualitatively or quantitatively. Qualitative analysis provides information about the nature of drugs, but quantitative analysis gives information about the chemistry and concentration of the drugs substances. Many of the researchers today apply computational intelligence techniques for forensic drug analysis, which employ those techniques for collecting and analyzing the sample data.

Table 1. Comparison of the general characteristics of forensic drug analysis.

	Presumptive Test	Confirmatory Test
Analysis Technique	Immunoassay	Gas Chromatography-Mass Spectrometry (GC-MS), Liquid Chromatography Mass Spectrometry (LC-MS)
Analysis	Qualitative	Quantitative
Sensitivity	Low	High
Cost	Low	High
Specificity	Low	High
Simplicity	Yes	No
Speed	Quick	Slow
Accuracy	Low	High

A. Screening Analysis

Screening analysis, also known as presumptive test is a preliminary step in a drug investigation to determine the present or absence of the illegal substances in the given suspected sample. The outcome of this presumptive test acts as a hypothesis for the investigation, which need to further confirm by the confirmatory analysis. Nonspecific instrumental analyses such as colorimetric and UV-visible spectrophotometric analyses may be used for qualitative analysis of toxins. Sophisticated techniques such as infrared spectroscopy, gas chromatography (GC), High Pressure Liquid Chromatography (HLPC), and immunoassay techniques may be employed to quantify the toxins.

1) Colorimetric Test

Colorimetric test is fast, economical, and easy to perform in presumptive forensic drug analysis. The test will indicate whether the suspected substance is present or absence by using color as an indicator. Color reaction is produced by detecting the presence of a particular chemical compound in the suspected sample. In [32], it provides a manual to establish the requirement for color test in forensic drug analysis.

2) Immunoassay techniques

Immunoassay technique is used to detect the presence of drugs and drug metabolites in a biological sample based on the principle of antibody-antigen reaction. It is a flexible

technique which provides fast, cost effective and convenient method to screen a large number of submitted samples in a variety of matrices [23]. There are few types of immunoassay methods that applied in the drug analysis: Radioimmunoassay, Enzyme Immunoassay, Fluoroimmunoassay, Chemiluminescence Immunoassay, and Liposome Immunoassay [24].

3) UV-visible spectrophotometric Test

This test obeys the Beer-Lambert law principle, which state that the greater the number of molecules to absorb light in a given wavelength, the greater the extent of a light absorption. This test is a measurement of the attenuation rate of a beam of light after it passes through an absorbing substance, is proportional to the incident radiation as well as the concentration of the solution. Beer's Law states that:

A = €bc, where € is a constant of proportionality, called the absorptivity.

A UV-visible spectrophotometric test can be applied in biochemistry and analytical chemistry to identify, quantify and purify the individual components of the substances. The reader may refer to [25] to get more detailed information about UV-visible spectrophotometric Test.

4) Infrared spectroscopy (IR)

Infrared Spectroscopy is the analysis of how the molecules reacting in particular regions of the electromagnetic spectrum. There are three main ways to analyze the reaction between the molecule and infrared light: absorption, emission and reflection. IR will measure the molecular motion, such as vibration, rotation, or combinations of these atoms to result in a change of the molecule's dipole moment. Generally, different functional group of the chemical compounds will result in different absorption, emission and reflection of frequencies and intensities on the infrared spectrum. Hence, based on this, IR may be used to identify and characterize the molecular compound in a mixture of substances.

5) Gas chromatography (GC)

GC is a technique that using a solid or a liquid coated on a solid support as a stationary phase (SP) and employing gas as a mobile phase (MP) to separate the volatile mixtures into constituent individual components. In gas chromatograph terminology, it divides into two phases which is stationary phase and mobile phase. The chromatographic column in the stationary phase is the component of the chromatograph where separation of compound occurs. It is coated onto the inner walls of a very narrow capillary called open tubular chromatography. Besides, the mobile phase is in the termed of carrier gas. This phase constantly moves over the stationary phase and both are in equilibrium.

6) High Pressure Liquid Chromatography (HPLC)

HPLC have the same underlying principle with the GS. Both of these techniques are used in the laboratory to separate the mixture of substances in a sample that injected into the SP. The significant difference between both these techniques are, HPLC uses a solid in SP and liquid in the MP while in the case of GC, compound in the mixture is separated using the liquid in the SP and uses gas as the carrier in the MP. HPLC has gained a high popularity in the field of pharmaceuticals, manufacturing, and research, whereas in GC has found favor in toxicology case, petroleum and petrochemical industry, environmental air monitoring and etc.

7) CI in Screening Analysis

An approach has been proposed for accelerated high-throughput drug screening and generalized protein-targeted drug discovery by using various tools with computational intelligence techniques such as evolutionary algorithm, evolved ANNs, docking software, and quantitative structure activity/property relationship (QSAR/QSPR) modeling. This proposed approach have been successfully tested on dihydrofolate reductase (DHFR) for novel antimalarial drug discovery [26].

An integration of structure-activity relationship couple with artificial intelligence systems have been applied to improve in-silico prediction of Ames Test Mutagenicity. The approach shown a good result with a lower error rate as compare to others predictive system and the system suitable for early determination of levels of genotoxicity concern [27].

(Richardson & Lidbury 2013), have constructed an ensemble-based classifier by bagging with the decision tree technique for pathology laboratory data, particularly to overcome a large imbalance of negative Hepatitis B virus (HBV) and Hepatitis C virus (HCV) cases versus HBV or HCV immunoassay positive cases. The authors is aiming to improve the laboratory diagnosis via informatics analyses.

In [29] paper, the authors have been proposed ANN technique to analyze and classify UV-visible spectra of mixtures of organic indicators. They successfully showed the significant result even with the presence of significant distortion in the spectral patterns. Their result suggest that the system is suitable for on-line monitoring of fabric defects at a high inspection rate.

(Kim et al. 2012), present a study that used an efficient grand canonical Monte Carlo (GCMC) simulations coupled with graphics processing units (GPUs) to perform a large-scale computational screening which aim to obtain the pure component adsorption isotherms from both ethane and ethene mixture. The result also proved that the optimal optimum ethane/ethene separation materials can be identified by screening framework geometries knowledge [30].

(Orelli et al. 2004), present a study to understand the critical condition used in the liquid chromatography by using lattice Monte Carlo simulation. The result that obtain in the study showed that it is inadequacy to use the Gaussian chain model to study the critical condition in liquid chromatography of polymers. Furthermore, it is required to use the excluded-volume chain coupled with Monte Carlo simulations to examine the partitioning of block, star, and ring polymers near the critical condition.

B. Confirmatory Analysis

In confirmatory analysis, the aim is to identify the specificity of the fingerprint that present in the submitted

material. It requires high sensitivity to determine what substances are present in the suspected substances. It requires a series of analytic instrumental test using techniques such as Gas Chromatograph-Mass Spectrometry (GC-MS), Liquid Chromatograph-Mass Spectrometry (GC-MS), or infrared spectroscopy that discretize the substance into the different individual compound and then analyze and interpret the result to identify the fingerprint present within the material.

1) Mass Spectrometry (MS)

Mass spectrometry is an instrument that used for separation and measurement the ionization of the molecules according to their mass to charge ratios (m/z). The output of this MS is to produce a typical pattern of ions which are used to identify the fingerprint of the molecules. It has high sensitivity and high specificity in identification of the therapeutic and illegal drugs, hence it is currently in wide use in the forensic drug analysis. Figure 4 below shows a state of the art flowchart of the MS components and it functions.

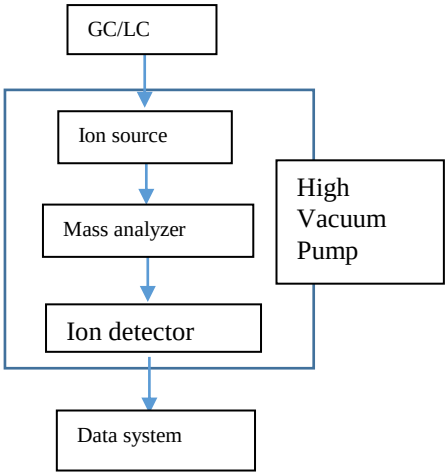

Figure. 4. MS Components and functions

2) CI in Confirmatory Analysis

(Ball et al. 2002), the authors have developed an integrated approach which utilising artificial neural networks and SELDI mass spectrometry for the classification of human tumours and rapid identification of potential biomarkers. They are successfully discriminated between multiple classes for blind data to identifying the biomarkers. The paper [35], the authors have been applied ANNs to a number of diverse areas for the identification of "biologically relevant" molecules, including pyrolysis mass spectrometry. In [36], ANN have been applied in neutron spectrometry and domestic problems for a bonner sphere spectrometer with a 3He detector. In [37], the authors have been developing a multi-layer perceptron (MLP) ANN approach specific to the analysis of MALDI mass spectrometry data. The authors have been proved that the proposed approach is robust and standardized, automated protocols for the model development process using mass spectrometry data from a wide area of domains.

(Khairallah et al. 2014) the authors have been proposed a mechanishm that combine both mass spectrometry and computation methodology into bimolecular gasphase reactions of peroxyl radicals with Phenylacetylene using the distonic radical ion approach. Spencer et al. (R. L. Spencer, J. Krogel, J. Palmer, A. Payne, A. Sampson 2009) have been developed a simulation of the flow of neutral argon gas through the first vacuum stage of the ICPMS by using Direct Simulation Monte Carlo (DSMC) algorithm.

(Wei et al. 2011) Introduces a novel computational platform for high-resolution mass spectrometry-based metabolomics: Metsign. It is a platform that using computational intelligence approaches to provide a suite of bioinformatics tools to perform raw data deconvolution, metabolite putative assignment, peak list alignment, normalization, statistical significance tests, unsupervised pattern recognition, and time course analysis. In addition, a study done in [41] to study an informatics methods that used to determine the presence of proteins and detecting the biomarker in LC-MS experiments.

IV. Conclusion

The molecular structure, as a complex structure, is akin to be fuzzy and evolutionary. In this paper, we have provided a brief overview of computational intelligence techniques and their application in the area of molecular structure application. Each computational intelligence technique is summarized and its utility to molecular structure application is analyzed. The paper consists of four main aspects: artificial neural network can learn complex nonlinear input-output relationships to improve the learning capability of the molecular structure; fuzzy logic summarize the domain knowledge with the use of symbol to deal with vagueness and uncertainty in molecular structure; genetic algorithm provides an efficient search methodology to deal with the vastness and tractability issues of molecular structure data; artificial neural network to improve the learning capability of the molecular structure; hybrid techniques combine one or more different techniques can give a robust solution to the problem at hand. Furthermore, we have briefly described the various tactics that used in the forensic drug analysis process that practice in laboratory by forensic chemist, and also review few key articles that have been successfully applied CI techniques in the forensic drug analysis process. We expect that this review will be of some assistance in the task of choosing the proper computational intelligence techniques for the application which involve identification of complex drug molecular structure.

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References

[1] Unodoc - UNITED NATIONS OFFICE ON DRUGS AND CRIME, “Recommended methods for the Identification and Analysis of Cocaine in Seized Materials,” *Unodoc*, 2012. .

[2] C. Darwin, “On the Origin of Species by Means of Natural Selection , or the Preservation of Favoured Races in the Struggle for Life.”

[3] D. B. FOGEL, “Theory of modern heuristic optimization,” pp. 1–24.

[4] J. Solomon, P. Chung, D. Srivastava, and E. Darve, “Method and advantages of genetic algorithms in parameterization of interatomic potentials: Metal oxides,” *Comput. Mater. Sci.*, vol. 81, pp. 453–465, 2014.

[5] P. Wałejko, K. Paradowska, J. Bukowicki, S. Witkowski, and I. Wawer, “Phenyl galactopyranosides – 13 C CPMAS NMR and conformational analysis using genetic algorithm,” vol. 457, pp. 43–50, 2015.

[6] Z. Li, J. Gu, H. Zhuang, L. Kang, X. Zhao, and Q. Guo, “Adaptive molecular docking method based on information entropy genetic algorithm,” *Appl. Soft Comput.*, vol. 26, pp. 299–302, 2015.

[7] T. Paul and H. Iba, “Identification of Informative Genes for Molecular Classification Using Probabilistic Model Building Genetic Algorithm,” *Genet. Evol. Comput. – GECCO 2004*, vol. 3102, pp. 414–425, 2004.

[8] a Harishchander, S. Senapati, and D. A. Anand, “Analysis of drug resistance to HIV-1 protease using fitness function in genetic algorithm,” vol. 12, no. Suppl 1, p. 2334, 2012.

[9] S. Haykin, “Neural Networks: A comprehensive foundation,” 1999.

[10] C. Lorenz, A. S. Ferraudo, and L. Suesdek, “Artificial Neural Network applied as a methodology of mosquito species identification,” *Acta Trop.*, vol. 152, pp. 165–169, 2015.

[11] Y. Li, M. R. Abbaspour, P. V. Grootendorst, A. M. Rauth, and X. Y. Wu, “Optimization of controlled release nanoparticle formulation of verapamil hydrochloride using artificial neural networks with genetic algorithm and response surface methodology,” *Eur. J. Pharm. Biopharm.*, vol. 94, pp. 170–179, 2015.

[12] W. Laosiritaworn and Y. Laosiritaworn, “Artificial Neural Network modeling of spin-transition behavior in two-dimensional molecular magnet: The learning by experiences analysis,” *Polyhedron*, vol. 66, pp. 108–115, 2013.

[13] A. R. Bahmani, F. Sabzi, and M. Bahmani, “Prediction of solubility of sulfur dioxide in ionic liquids using artificial neural network,” *J. Mol. Liq.*, vol. 211, pp. 395–400, 2015.

[14] A. Ghaedi, “Simultaneous prediction of the thermodynamic properties of aqueous solution of ethylene glycol monoethyl ether using artificial neural network,” *J. Mol. Liq.*, vol. 207, pp. 327–333, 2015.

[15] Zadeh, “Fuzzy Sets-Information and Control-1965.” pp. 338–353, 1965.

[16] S. Vijayakumar and P. T. V Lakshmi, “A fuzzy inference system for predicting allergenicity and allergic cross-reactivity in proteins,” *Proc. - 2013 IEEE Int. Conf. Bioinforma. Biomed. IEEE BIBM 2013*, no. Mlc, pp. 49–52, 2013.

[17] Y. S. Y. Sun, G. F. G. Feng, and J. C. J. Cao, “A New Approach to Dynamic Fuzzy Modeling of Genetic Regulatory Networks,” *IEEE Trans. Nanobioscience*, vol. 9, no. 4, pp. 263–272, 2010.

[18] C. Umoja, E. A. Durham, A. Rosen, and R. W. Harrison, “A Novel Approach to Determine Docking Locations Using Fuzzy Logic and Shape Determination,” pp. 31–33, 2014.

[19] S. D. K. A. Theofilatos, C. M. Dimitrakopoulos, A. K. Tsakalidis and S. P. M. Likothanassis, S. T. Papadimitriou, “A New Hybrid Method for Predicting Protein Interactions Using Genetic Algorithms and Extended Kalman Filters,” pp. 0–3, 2010.

[20] R. Boiocchi, M. Mauricio-Iglesias, a. K. Vangsgaard, K. V. Gernaey, and G. Sin, “Aeration control by monitoring the microbiological activity using fuzzy logic diagnosis and control. Application to a complete autotrophic nitrogen removal reactor,” *J. Process Control*, vol. 30, pp. 22–33, 2014.

[21] M. E. Hamzehie and H. Najibi, “Prediction of carbon dioxide loading capacity in amino acid salt solutions as new absorbents using artificial neural network and Deshmukh–Mather models,” *J. Nat. Gas Sci. Eng.*, 2015.

[22] N. Geçen, E. SarIpInar, E. Yanmaz, and K. Şahin, “Application of electron conformational-genetic algorithm approach to 1,4-dihydropyridines as calcium channel antagonists: Pharmacophore identification and bioactivity prediction,” *J. Mol. Model.*, vol. 18, no. 1, pp. 65–82, 2012.

[23] D. Testing, “Drug Testing David Cowan University of London David Osselton Forensic Science Service Steven Robinson,” *Science (80-.).*

[24] I. A. Darwish, “Immunoassay Methods and their Applications in Pharmaceutical Analysis: Basic Methodology and Recent Advances.,” *Int. J. Biomed. Sci.*, vol. 2, no. 3, pp. 217–35, Sep. 2006.

[25] A. Thakur, “Principle, working and applications of UV spectroscopy,” 2011. [Online]. Available:http://www.indiastudychannel.com/resources/146681-Principle-working-and-applications-of-UV-spectroscopy.aspx. [Accessed: 27-Jan-2016].

[26] D. Hecht and G. B. Fogel, “A novel in silico approach to drug discovery via computational intelligence,” *J. Chem. Inf. Model.*, vol. 49, no. 4, pp. 1105–1121, 2009.

[27] P. Mazzatorta, L.-A. Tran, B. Schilter, and M. Grigorov, “Integration of structure-activity relationship and artificial intelligence systems to improve in silico prediction of ames test mutagenicity.,” *J. Chem. Inf. Model.*, vol. 47, no. 1, pp. 34–8, 2007.

[28] A. M. Richardson and B. A. Lidbury, “Infection status outcome, machine learning method and virus type interact to affect the optimised prediction of hepatitis virus immunoassay results from routine pathology laboratory assays in unbalanced data.,” *BMC Bioinformatics*, vol. 14, no. 1, pp. 206 – 213, 2013.

[29] A. D. A. Tilocca, P. Borzone, S. Carosio, “Detecting Fabric Defects with a Neural Network Using Two Kinds of Optical Patterns,” 2002.

[30] J. Kim, L. C. Lin, R. L. Martin, J. a. Swisher, M. Haranczyk, and B. Smit, “Large-scale computational screening of zeolites for ethane/ethene separation,” *Langmuir*, vol. 28, no. 32, pp. 11914–11919, 2012.

[31] S. Orelli, W. Jiang, and Y. Wang, “A computational Investigation of the Critical Condition Used in the Liquid Chromatography of Polymers,” *Macromolecules*, vol. 37, pp. 10073–10078, 2004.

[32] N. I. of Justice, “Color Test Reagents/Kits for Preliminary Identification of Drugs of Abuse,” *NIJ Stand.*, p. 19, 2000.

[33] G. Ball, S. Mian, F. Holding, R. O. Allibone, J. Lowe, S. Ali, G. Li, S. Mccardle, I. O. Ellis, C. Creaser, and R. C. Rees, “An integrated approach utilizing artificial neural networks and SELDI mass spectrometry for the classification of human tumours and rapid identification of potential biomarkers,” *Bioinformatics*, vol. 18, no. 3, pp. 395–404, 2002.

[34] M. Chun, J., Atalan, E., Ward, A. C. & Goodfellow, “Artificial neural network analysis of pyrolysis mass spectrometric data in the identification of Streptomyces strains,” *FEMS Microbiol Lett*, pp. 321–325, 1993.

[35] J. M. Ort, “Neutron spectrometry using artificial neural networks for a bonner sphere spectrometer with a 3 He detector,” vol. 57, no. 1, pp. 69–71, 2011.

[36] B. Matharoo-ball, J. Garibaldi, R. Rees, N. Kalsheker, K. Morgan, and G. Ball, “Computational Methods For The Diagnosis Of Alzheimer ’ S Disease From Cerebro-Spinal Fluid Bymatrix

Assisted Laser Desorption-Ionisation Mass Spectrometry (MALDI-MS)."
[37] G. N. Khairallah, R. A. J. O'Hair, and U. Wille, "Mass Spectrometric and Computational Studies on the Reaction of Aromatic Peroxyl Radicals with Phenylacetylene Using the Distonic Radical Ion Approach," *J. Phys. Chem. A*, vol. 118, no. 18, pp. 3295–3306, 2014.
[38] W. S. and C. N. W. R. L. Spencer, J. Krogel, J. Palmer, A. Payne, A. Sampson, "Modeling the gas flow upstream and in the sampling nozzle of the inductively cou-pled plasma mass spectrometer via the Direct Simulation Monte Carlo algorithm, Spectrochim," vol. 64, pp. 215–221, 2009.
[39] X. Wei, W. Sun, X. Shi, I. Koo, B. Wang, J. Zhang, X. Yin, Y. Tang, B. Bogdanov, S. Kim, Z. Zhou, C. McClain, and X. Zhang, "MetSign: A Computational Platform for High-Resolution Mass Spectrometry-Based Metabolomics," *Anal. Chem.*, vol. 83, no. 20, pp. 7668–7675, 2011.
[40] D. Radulovic, S. Jelveh, S. Ryu, T. G. Hamilton, E. Foss, Y. Mao, and A. Emili, "Informatics platform for global proteomic profiling and biomarker discovery using liquid chromatography-tandem mass spectrometry.," *Mol. Cell. Proteomics*, vol. 3, no. 10, pp. 984–97, Oct. 2004.
[41] K. Jeong, M. Kim, H. Jo, J. Gim, D. Kim, and G. Joo, "Ecological Informatics Search of optimal locations for species- or group-speci fi c primer design in DNA sequences : Non-dominated Sorting Genetic Algorithm II (NSGA-II)," Ecol. Inform., vol. 29, pp. 214–220, 2015.
[42] S. Deng, W. Su, and L. Zhao, "A neural network for predicting normal boiling point of pure refrigerants using molecular Un réseau neuronal pour prédire le point d ' ébullition normal de purs frigorig ènes en utilisant les groupes mol éculaires et un indice topologique," vol. 63, pp. 63–71, 2016.
[43] N. Murilo, N. Lima, L. Zu, F. Manenti, R. Maciel, M. Regina, W. Maciel, M. Embiruc, and L. Carmen, "Chemical Engineering Research and Design," vol. 9, no. July, pp. 471–479, 2010.

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