

PATTERN RECOGNITION OF AMPHETAMINES FTIR SPECTRA WITH MODIFIED PHASE-INPUT FOURIER CORRELATION

Alin C. Teusdea¹, Mirela Praisler²

¹University of Oradea, Faculty of Environmental Protection, Gen. Magheru 26, Oradea 410058, BH, Romania

²“Dunarea de Jos” University of Galati, Faculty of Sciences, Domneasca 47, Galati 800008, GL, Romania

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Abstract

This paper presents a pattern recognition analysis over a database of GC-FTIR spectra of pure amphetamines ($3745\text{-}605\text{cm}^{-1}$). The analyzed spectra are organized in three classes: stimulant amphetamines (15 spectra), hallucinogenic amphetamines (7 spectra) and non-amphetamines (135 spectra).

The correlation process is based on amplitude sine modulated fringe-adjusted phase-input joint transform correlation method (FA-sinePiJTC). In this method, the correlation is done between a pair of phase-transformed amphetamines spectra. The proposed phase-input algorithm consists of two steps: the amplitude sine modulation step and the adaptive filtering step.

The results show that all the correlations coefficients corresponding to the 157×157 correlation matrix are above the detection efficiency coefficient threshold value of 1,2000. In conclusion, the pattern recognition method based on modified phase-input Fourier correlation is adequate for the discrimination of the GC- FTIR spectra of amphetamines.

1. Introduction

Pattern recognition is an imposed step in the classification of chemical compounds, based on their spectral behaviour. Worldwide, the amphetamines are monitored by the security agencies due to the important number of analogues that are used as drugs of abuse (e.g. hallucinogens). On the other hand, some amphetamine analogues with stimulant biological effect are used in legal medical applications. As a result, their discrimination from non-amphetamine molecular structures or classification (stimulant amphetamines vs. hallucinogenic amphetamines) is somehow critical, especially if it can be done automatically. One way to obtain their classification is to build up a GC-FTIR spectral database and then to design a pattern recognition algorithm that can distinguish the class identity of an unknown molecular structure.

The forensic practice requires the positive identification of an illicit amphetamine based on both its GC-MS and GC-FTIR spectrum. The challenge in achieving the automated recognition of the class identity of these compounds is the fact that the different amphetamine analogues have very similar molecular structures and thus their spectra are very similar as well. This is especially true for the GC-MS spectra, fact that generates the failure of the pattern recognition process at the levels of sensitivity and selectivity required by the forensic practice. The GC-FTIR spectra are more sensitive to small changes in the molecular structure, and thus have been selected for this study.

Amplitude fringe-adjusted joint transform correlator [1, 2], FA-AJTC, is a well known pattern recognition tool. However, a preliminary study has shown that, despite the advantage of noise robustness, it is not powerful enough to discriminate the amphetamines spectra. This is the reason why we have analysed the results obtained with the sine modulated phase-input joint transform correlator (FA-sinePiJTC) in the pattern recognition process designed to identify the class identity of the amphetamines based on their GC-FTIR spectra. For a better understanding of the benefits of FA-sinePiJTC, we are presenting in the following sections the transitions from the FA-AJTC to the proposed one.

2. Method and samples

2.1. Fringe adjusted amplitude joint transform correlator (FA-AJTC)

Let us assume that we have a scene-function $scn(x - x_0)$ and a reference-function $ref(x + x_0)$ as the input function, separated by a distance of $2x_0$ along the x-axis. Thus we obtain a joint image function

$$jnt(x) = ref(x + x_0) + scn(x - x_0). \quad (1)$$

The Fourier transform of expression (1), given by [1-3]

$$Jnt(u) = Ref(u) \cdot \exp(iux_0) + Scn(u) \cdot \exp(-iux_0), \quad (2)$$

where $Jnt(u)$, $Ref(u)$ and $Scn(u)$ are the Fourier transforms of $jnt(x)$, $ref(x)$ and $scn(x)$, respectively, and $u = 2\pi \cdot x$ is the coordinate in the Fourier space. The joint power spectrum in the Fourier space is given by [1, 2]

$$JPS(u) = RPS(u) + SPS(u) + REF^*(u) \cdot SCN^*(u) \exp(iu \cdot 2x_0) + SCN(u) \cdot REF^*(u) \exp(-iu \cdot 2x_0). \quad (3)$$

Then the joint power spectrum, from Fourier space, is inverse transformed to obtain the correlation information as the output function, which is given by

$$\begin{aligned} Corr(x) &= [ref(x) \otimes ref(x) + scn(x) \otimes scn(x)] + ref(x) \otimes scn(x + 2x_0) + scn(x) \otimes ref(x - 2x_0) \\ &\equiv T_0 + T_1 + T_2 \end{aligned} \quad (4)$$

where the \otimes symbol denotes the correlation operation. The T_0 term, in expression (4), denotes the zero-order term, which consists of autocorrelation peaks for the reference and the input functions, located in the centre of the output function. The T_1 and T_2 terms represent the two correlation peaks that are the useful signals for the recognition information.

One major problem of the correlator is that after the correlation process is performed a very high term occurs in the output function, the dc term. The dc term has to be removed in order to enable the examination of the correlation useful peaks. One way is done in the first Fourier space, where the non-zero order power spectrum is obtained by [1, 2]

$$JnzPS(u) = JPS(u) - SPS(u) - RPS(u) . \quad (5)$$

Furthermore to improve the pattern discriminability of the correlation process the cross-correlation peaks must be reduced and the autocorrelation peaks increased. This adjusting can be done by applying an amplitude-modulated filter $Flt(u)$ to the non-zero order joint power spectrum. The amplitude adjusting filter is defined by [1, 2]

$$Flt(u) = \begin{cases} 1/[REF(u)], & REF(u) > \varepsilon \\ 1/[REF(u) + Z(u)], & REF(u) \leq \varepsilon \end{cases} , \quad (6)$$

where ε is the lowest real positive value that the computer recognizes, and $Z(u)$ is a real non-zero function. In the first Fourier space the fringe-adjusted function is

$$H(u) = Flt(u) \cdot JnzPS(u) . \quad (7)$$

Finally, in order to obtain the correlation peaks, this function will be Fourier transformed. The fringe-adjusted amplitude joint transform correlator (FA-AJTC) is the correlator that provides this kind of correlation process, equations (5) to (7).

2. 2. Fringe-adjusted phase-input joint transform correlator (FA-PiJTC)

This correlator model is the same as the amplitude one, but it uses the phase transformation method on the joint input image. This method assumes that the input amplitude function, $AmpFunc(x)$, is somehow transformed from amplitude coding in phase coding

(usually $dfPSLM \equiv \pi$ and $dfPSLM \equiv 2\pi$), using a transformation function $Tf[\cdot]$ to obtain a phase-input function $PhaseFunc(x)$, that mathematically is described by [3-9]

$$PhaseFunc(x) = \exp\left[i \cdot Tf[AmpFunc(x)]\right] = \exp\left[i \cdot \left(\frac{AmpFunc(x) - Min}{Max - Min}\right) \cdot dfPSLM\right], \quad (8)$$

where $dfPSLM$ is the phase depth, Max , Min , are the maximum and the minimum values of the amplitude input function. After the phase transformation of reference, scene and joint images, the entire process works identically like in the FA-AJTC.

2.3. Sine modulated fringe-adjusted phase-input joint transform correlator (FA-sinePiJTC)

The phase-input joint transform correlator FA-PiJTC is reported to be noise sensitive. In certain conditions a better pattern discriminability and better detection efficiency is needed. The detection efficiency can be improved if the dc term (which is the zero order term) of the power spectrum will drop and the high spatial frequencies will increase.

The high spatial frequencies are connected to the function's details in spatial coordinates. If the three power spectrum will have a thin dc term and large high spatial frequencies, the correlation process, which "compares" the reference function with the scene objects, will provide a better pattern discrimination because the objects will be "compared" more in their details.

To achieve this goal the authors propose an alternate correlator, which consists in applying a sine function before the first Fourier transform is performed:

$$PhaseFunc(x) = \exp\left[i \cdot \left[\sin\left(\left(\frac{AmpFunc(x) - Min}{Max - Min}\right) \cdot dfPRE + fPRE_1\right)\right] \cdot dfPSLM\right]. \quad (9)$$

where $dfPRE = fPRE_2 - fPRE_1$ is the amplitude sine modulation domain. The amplitude sine modulation function reshapes the input functions such as the minor details differences becomes larger differences. Thus are generate large high frequencies and pattern recognition efficiency.

After this proposed phase transformation of the input function, the previous algorithm can be performed. The sine modulated fringe-adjusted phase-input joint transform correlator (FA-sinePiJTC) is the correlator that provides this kind of correlation process, equations (5) to (7) and equation (9).

3. Results and Discussions

The database that was used as input for the pattern recognition process consists of 157 GC-FTIR spectra recorded in the $3745\text{-}605\text{ cm}^{-1}$ spectral domain. The spectra are organized in three classes: stimulant amphetamines, hallucinogenic amphetamines and non-amphetamines. Despite the presence of the three amphetamines classes, the authors considered just one class of amphetamines, regardless of their biological activity. The resulting data will provide the pattern recognition parameters which are needed for any further, more refined, automated classification tools.

The pattern recognition process was done with the FA-sinePiJTC. The result was a 157×157 correlation matrix with the detection efficiency coefficient values.

The correlation performances criteria that can be used to analyse the described joint transform correlators need the definition of the cross-correlation peak intensity, CPI, and of the auto-correlation peak intensity, API. The ratio, $DEC = API/CPI$, denotes the detection efficiency coefficient. It prescribes a pattern recognition failure for values less than the recommended threshold value of 1,2000. Values greater than the threshold conclude in a successful pattern recognition process.

The used parameters with FA-sinePiJTC were $dfPSLM \equiv [2\pi - 0]$ and $dfPRE = [(3\pi) - (-0.5\pi)]$. Correlation results from pattern recognition process made with objects from a database are summarized by the minimum value of the detection efficiency coefficient, DEC_{min} .

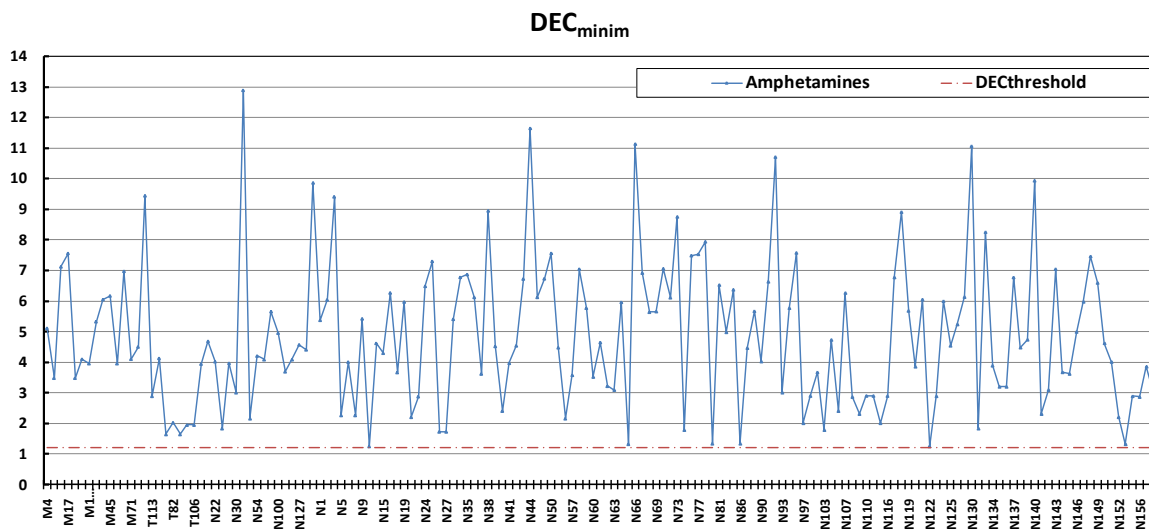


Figure 1. Fourier correlation results for the three amphetamines classes.

The minimum DEC value for a pattern recognition process for one reference object over the rest is characterized by the “worst” correlation result. Figure 1 shows the graphical representations of the pattern recognition results with the FA-sinePiJTC for the three analysed classes. The DEC_{min} values are represented for each GC-FTIR amphetamine spectrum over the rest. The dash dotted line represents the detection efficiency coefficient threshold value.

First, the FA-sinePiJTC generates the amplitude sine modulated input function (i.e. the spectra of amphetamines). This procedure increases the differences between the discriminated spectra involved in the correlation process. A second data processing step yields the fringe-adjusted power spectrum, which has the effect of reference adaptive filtering. In this way, the discriminability between the amphetamines spectra increases in comparison with the other two joint transform correlators.

The final correlation results, represented by the DEC_{min} values, are compared with the threshold value of the correlation coefficient, that was set at 1,2000. Table 1 presents the overall DEC_{min} values that were obtained for the studied classes of amphetamines. The non amphetamines class generates the lowest DEC_{min} value for the N10 and N122 indexed pair.

Table 1. Minimum values of detection efficiency coefficient for the studied three amphetamines classes.

Amphetamines Class	DEC_{minim}
Stimulant	3.4723
Halucinogen	1.6299
Non-Amphetamines	1.2385

This means that these two GC-FTIR spectra of non-amphetamines are very similar (the Pearson correlation coefficient is 0.9857 or the equivalent $DEC = 1.0145$). Despite this situation, the FA-sinePiJTC can discriminate N10 and N122 with a DEC “gap” value of 0.0385 (3.208%) above the DEC threshold value.

Conclusions

In this paper we have presented the classification results obtained with the sine modulated fringe-adjusted phase-input joint transform correlator, FA-sinePiJTC, and its benefits in pattern recognition of pure amphetamines, based on the processing of their GC-FTIR spectra.

The above results reach the conclusion that the presented pattern recognition method based on the sine modulated fringe-adjusted phase-input joint transform correlator, FA-sinePIJTC, is adequate for assigning the class identity of amphetamines based on their GC-FTIR spectra. Furthermore, the DEC “gap” between threshold value and DEC_{\min} is large enough to consider this method recommendable for both the registration and classification tasks required for the automated recognition of GC-FTIR spectra of pure amphetamines.

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