Application of Revised Version of Neural Independent Component Analysis to Classification Problems of Confiscated Methamphetamine

Tatsuya TAKAGI,*[,a,b] Yukiko MAKINO,[c] Yuko TANAKA,[a] Kousuke OKAMOTO,[a] Noriyuki YAMASHITA,[a] Tomoko MATSUMOTO,[d] Masahiko YOKOTA,[a] Ken KUROKAWA,[b,e] and Teruo YASUNAGA[b]

[a] *Graduate School of Pharmaceutical Sciences, Osaka University; 1–6 Yamadaoka, Suita, Osaka 565–0871, Japan:* [b] *Genome Information Research Center, Osaka University; 3–1 Yamadaoka, Suita, Osaka 565–0871, Japan:* [c] *Narcotics Control Department, Kanto-Shin'etsu Bureau of Health and Welfare, Ministry of Health, Labor and Welfare; 2–4–14 Nakameguro, Meguro-ku, Tokyo 153–0061, Japan:* [d] *Faculty of Pharmaceutical Sciences, Osaka University; 1–6 Yamadaoka, Suita, Osaka 565–0871, Japan: and* [e] *Research Institute of Microbial Diseases, Osaka University; 3–1 Yamadaoka, Suita, Osaka 565–0871, Japan.*

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Recently, profiling the chemical substances in illegally distributed drugs has been needed in order to reveal the drug channels. However, this kind of profiling is often difficult because such drugs contain various kinds of impurities and the quantity of these impurities changes. Due to these circumstances, several methods, including a slightly revised ICA (Independent Component Analysis) by a Hebbian learning artificial neural network, were applied for profiling illegally distributed methamphetamine. Eventually, better classification results with the ICA than with other methods were obtained. These results show that ICA could make it easier to profile illegally distributed methamphetamine.

Key words independent component analysis; methamphetamine; confiscated drug; hebbian learning; artificial neural network

In Japan as well as in many other countries, drugs of abuse have become a more serious problem. Because of the drastic changes in the political situation in the Middle East and the Korean Peninsula, especially during the last few years, a prompt and adequate response has been required against the illegal distribution of drugs. One response is the U.N.-led support of surveillance systems, and so on, which could help curb the illegal distribution of drugs. However, the channels of illegal distribution of drugs of abuse have also changed in the last few years, and this change affects the methods of action against the illegal distribution of drugs.

Under these circumstances, profiling the chemical substances in illegally distributed drugs is needed in order to reveal the drug channels. However, this kind of profiling, which includes the impurities in the drugs, is often difficult because such drugs contain various kinds of impurities and the quantity of these impurities changes. Therefore, there have only been a few studies on impurity analyses using such multivariate analyses as the cluster analysis, SIMCA[1] (Soft Independent Modeling of Class Analogy), and PCA (Principal Component Analysis). For example, Strömberg *et al.*[2] applied SIMCA and PCA, and Neumann[3] applied cluster analysis for profiling heroin using general classification (GC) data. Nevertheless, no methods could adequately succeed in classifying and profiling heroin. In any case, it was not shown whether these multivariate statistical methods had enough capability to profile drugs of abuse. Recently, independent component analysis (ICA)[4] has become more common in the field of signal analyses; this method is often used for solving blind source separation (BSS) problems. However, there have been few studies in the fields of chemistry and pharmaceutical sciences in which ICA has been applied, even though ICA is expected to be a classification and profiling method in such fields.

In this study, we applied an ICA using a Hebbian learning artificial neural network, which was first proposed by Oja *et al.*[5—7] We slightly revised Oja's ICA for profiling illegally distributed methamphetamine. Eventually, we obtained better classification results than with other methods. These results show that ICA could make it easier to profile illegally distributed methamphetamine.

Experimental

Methods ICA: ICA was initially developed in the field of signal analysis for revealing original signals from mixed signals with a lot of noise. Let $s_i(t)$ ($i=1, 2, \ldots, m$) be the i-th independent signal which is generated from m signal sources and $\xi_j(t)$ ($j=1, 2, \ldots, m$) be the j-th observed signal at m observation points (Fig. 1). $\xi_j(t)$ is expressed as follows:

$$\xi_j(t)=\sum_{i=1}^{m} a_{ij}s_i(t) \tag{1}$$

$$\boldsymbol{\xi}(t)=\mathbf{A}\mathbf{s}(t) \tag{2}$$

Here, $\mathbf{A}=\{a_{ij}\}$ is a transformation matrix, $\boldsymbol{\xi}(t)=\{\xi_1(t), \xi_2(t), \ldots, \xi_m(t)\}$, and $\mathbf{s}(t)=\{s_1(t), s_2(t), \ldots, s_m(t)\}$. As an example, one of the problems which can be solved using ICA is BSS. To solve BSS, $\mathbf{s}(t)$ has to be obtained from $\boldsymbol{\xi}(t)$; in other words, the regular matrix, $\mathbf{A}$, has to be obtained. However, since $\mathbf{A}$ cannot be determined uniformly, $\boldsymbol{\psi}(t)$, that is, $\mathbf{B}$, as in

$$\boldsymbol{\psi}(t)=\mathbf{B}\boldsymbol{\xi}(t) \tag{3}$$

should be obtained instead of $\mathbf{A}$ under the qualification that the original signals do not follow a normal distribution, whereas the mixed signal, $\xi(t)$, does tend to follow a normal distribution. Thus, based on the maximization of non-normality, $\mathbf{s}(t)$ can be obtained.

Very recently, a few studies[5,6] have been carried out on the artificial neural network (ANN) methods used for obtaining the separated signals, $\mathbf{s}(t)$. For example, Oja *et al.*[5—7] applied Hebbian learning ANN for BSS, and Brát *et al.*[8] adopted a self-organizing map (SOM) with PCA for the same purpose. Using $\mathbf{w}$ as the weight vector and $\mathbf{x}$ as the input data of a neuron, Oja's algorithm is as follows:

$$\begin{aligned}\mathbf{W}(t+1)=\mathbf{W}(t)+\mu(t)\mathbf{x}(t)f(\mathbf{x}(t)^T\mathbf{W}(t))\mathrm{diag}(\mathrm{sign}(c_i(t)))\\ +\alpha\mathbf{W}(t)(\mathbf{I}-\mathbf{W}(t)^T\mathbf{W}(t))\end{aligned} \tag{4}$$

where α is a constant, $\mu(t)$ is the ordinary learning ratio at the t-th learning, $\mathbf{W}(t)$ is the weight matrix whose columns are the weight vectors, $\mathbf{w}(t)$, of the

* To whom correspondence should be addressed. e-mail: ttakagi@phs.osaka-u.ac.jp

Table 1. Equations Used for Generating Test Data Sets

	Equations
Data-1	$z_1 = 0.1x_1^2 + 0.2x_1 + 0.3x_2^3 + 0.4x_3^2 + 0.5\sqrt[4]{x_4^2} - 0.2\sqrt[4]{x_5^2} + 0.7x_5 - 0.2$
	$z_2 = -0.2\sqrt[4]{x_1^2} - 0.3x_1 - 0.4\sqrt[4]{x_2^2} + 0.1\sqrt[4]{x_3^2} + 0.2x_4^2 + 0.3x_5^2 + 0.4x_5 + 0.1$
Data-2	$z_1 = 0.1x_1^2 - 0.5x_1 - 0.2x_2^3 + 0.3x_3^2 + 0.1\exp(x_4) - 0.5\sqrt[4]{x_5^2} - 0.2x_5 + 0.1$
	$z_2 = -0.1\sqrt[4]{x_1^2} + 0.2x_1 - 0.5\exp(x_2) + 0.7\exp(x_3) - 0.2x_4^2 + 0.1x_5^2 + 0.3x_5 - 0.2$

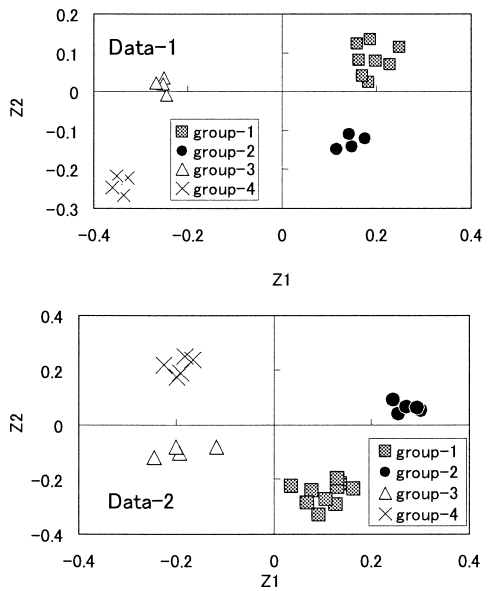

Fig. 1. Plot of Generated Data Sets

The four groups were arbitrarily determined so that the capabilities of the five classification methods could be visually revealed.

neurons, $f(\ldots)$ is the learning function, which can be different for each neuron, and the values of $c_i(t)$ ($i=1, 2, \ldots, n$) are estimated according to Eq. 5:

$$\Delta c \propto [\mathbf{w}^T\mathbf{x} f(\mathbf{w}^T\mathbf{x}) - f'(\mathbf{w}^T\mathbf{x})] - c$$
$$c(t+1) = c(t) + \beta|[\mathbf{w}^T(t)\mathbf{x}(t) f(\mathbf{w}(t)^T\mathbf{x}(t)) - f'(\mathbf{w}^T(t)\mathbf{x}(t))] - c(t)| \quad (5)$$

In order to make a more flexible system, we use a slightly revised version of Oja's method. Although Oja *et al.*[5—7] adopted only one learning function for each neuron, we adopted three functions,

$$f_1(x) = \tanh(2x)$$
$$f_2(x) = \sin(\pi x) \quad (6)$$
$$f_3(x) = \exp\{-3\exp(x^2)\}$$

Oja's original method was followed for other details.

Other Methods: In order to compare the results of the classification of confiscated methamphetamine using the revised neural ICA method, other statistical classification methods were applied. We adopted four additional methods: principal component analysis (PCA), categorical PCA (CATPCA),[9] metric multidimensional scaling method (MDS), and nonlinear principal component analysis using a five-layer hierarchical neural network (HNN). For the metric MDS computation, PROXSCAL[10] with Euclidean distances was used throughout this study. Although other options such as non-metric MDS were adopted, better MDS classification results were not obtained.

Data Artificial Data: Before applying the ICA to the profiling of confiscated methamphetamine, we prepared and applied several artificial data sets to confirm that ICA could be used. Since most of them could not be classified adequately by any methods, we selected the two data sets that could be classified adequately by some methods. In order to prepare the data sets, predictable variables, x_i ($i=1, 2, \ldots, n$; $-0.5 < x_i = 0.5$) were generated using a random number generator. Subsequently, according to the equations shown in Table 1, the z_{ji} ($i=1, 2, \ldots, n$; $j=1, 2$) values were calculated for the classifications using the five data mining methods. From the many data points generated using these equations, 20 data points were selected so that several groups, which consisted of 4—9 data points, could be visually classified from the scatter plots between z_1 and z_2. The two data sets are shown in Fig. 1 and Table 2. In order to clarify the capabilities of the abovementioned five classification methods, the 20 data in Fig. 1 were arbitrarily classified into four groups, that is, groups 1—4. Although these z_{ji} values are not the answers of the multivariate analyses, they indicate that clear classification results can be obtained if the method has the capability to solve nonlinear relations between predictable variables.

GC-MS Data of Confiscated Methamphetamine: The data for the impurity analysis of the confiscated drugs were obtained from the 109 peak areas of the GC-MS (gas chromatograph-mass spectrometry) spectra of 50 samples.

A GC-MS equipped with a Hewlett-Packard (HP) 6890 series gas chromatograph, a double-focusing mass spectrometer Mstation (JEOL, Tokyo, Japan), and a data processing XMS system (JEOL, Tokyo, Japan) were used for the profiling of methamphetamine crystals. An Ultra-2 fused-silica capillary column (30 m×0.2 mm×0.33 μm, HP) was inserted directly into the ion source of the mass spectrometer, and the analysis was performed in the splitless mode with helium as the carrier gas. The GC program was run from 50 °C (1 min) to 300 °C (4 min) at 10 °C/min, with the injection port at 250 °C. Electron-impact ionization mass conditions were set as follows: ionizing energy, 70 eV; ionization current, 300 μA; and ion-source temperature, 300 °C. Mass spectra were obtained using the scanning mode.

A sample of 50 mg of seized methamphetamine hydrochloride was dissolved in 1 ml of 0.1 M phosphate buffer (pH 7.0). The solution was made basic with 0.25 ml of 10% Na_2CO_3 and extracted by vigorous shaking for 5 min. with 0.4 ml of ethyl acetate containing triacontane (C30: 0.05 mg/dm^3) as an internal standard. After centrifugation, the organic layer was transferred with a Pasteur pipette into the insert of a microvial (Agilent Technologies) for the auto-sampler.

These drugs were confiscated in Australia, China, Czech Republic, Korea, Sweden, and the U.S.A. In addition, the GC-MS data of the synthesized methamphetamine[11] through four routes—the Emde method, reductive amination method, Leuckart method, and Nagai method—were added to the data of the confiscated methamphetamine to clarify the profiling results because the types of impurities included in synthesized methamphetamine depend upon the synthesis routes.[11] In order to perform the profiling analyses more easily, the data values were standardized as follows. 1) Let x_{ij} ($i=1, 2, \ldots, n$; $j=1, 2, \ldots, m$) be a peak area of a certain peak of the GC-MS spectra. Here, i means a certain peak and j means a certain confiscated methamphetamine. 2) Calculate ξ_{ij} according to the equation, $\xi_{ij} = \ln x_{ij}$. 3) Obtain the ξ_{ij} that means a standardized value of ξ_{ij} according to Eq. 7.

$$\zeta_{ij} = \frac{\xi_{ij} - \bar{\xi}_j}{s_j}$$
$$\bar{\xi}_j = \frac{1}{n}\sum_{i=1}^{n}\xi_{ij} \quad (7)$$
$$s_j = \frac{1}{n-1}\sqrt{\sum_{i=1}^{n}(\xi_{ij} - \bar{\xi}_j)^2}$$

4) Obtain the ζ'_{ij} that means a standardized value of ζ_{ij} according to Eq. 8.

Table 2. Artificial Data Prepared for the Test of Classification Capability

Data-1				
x_1	x_2	x_3	x_4	x_5
−0.20701	−0.21832	−0.36394	−0.44746	0.268734
−0.34165	0.474587	−0.29539	−0.22833	0.381267
−0.405	0.283235	0.436673	0.35734	0.225838
0.06837	0.249905	0.101327	−0.08189	0.49789
−0.42799	0.451463	−0.39625	0.249207	0.255345
−0.23435	0.278672	−0.37635	−0.29738	0.216025
−0.31734	0.20907	0.067674	0.419557	0.254287
−0.25768	0.127402	0.00681	−0.32771	0.324493
0.262454	0.34542	0.159079	0.10656	0.312985
0.339718	0.159599	0.210677	−0.15341	0.191969
0.342078	0.333982	−0.17756	0.019305	0.387182
0.308362	0.214837	−0.29699	0.091783	0.185042
−0.48599	−0.07108	−0.32558	0.238161	−0.23261
−0.4926	−0.02537	−0.39578	−0.20487	−0.23863
−0.01963	0.008388	0.16639	−0.09194	−0.17949
−0.00405	0.008022	−0.42883	0.21646	−0.35973
−0.31893	−0.42415	0.246367	0.355744	−0.45048
-0.20612	0.482067	0.164497	0.311755	−0.46201
−0.31793	0.409904	0.451488	−0.14583	−0.41632
−0.03759	−0.41198	−0.23293	0.149557	−0.41433
Data-2				
x_1	x_2	x_3	x_4	x_5
−0.2021	−0.03555	−0.33049	0.091978	0.106592
0.008989	0.06679	−0.27002	−0.06515	−0.02541
−0.3136	−0.09888	−0.31037	−0.32284	0.166866
−0.32663	−0.03775	0.011404	−0.21028	−0.34592
−0.25038	−0.20467	−0.27468	0.132957	−0.4383
−0.25931	0.149581	−0.17606	−0.30146	0.136903
−0.14049	0.028399	−0.30077	−0.07372	−0.24882
−0.06433	0.032074	−0.21303	−0.33926	−0.10254
−0.04386	0.061687	−0.3787	−0.39036	0.08541
−0.19785	−0.28989	−0.17933	−0.43633	−0.44766
−0.4803	−0.20351	0.143248	−0.36877	0.107332
−0.28048	0.199942	0.416594	0.159459	−0.16767
−0.45727	−0.08488	0.199582	−0.11482	0.10039
−0.33485	0.266735	0.39208	0.407016	0.092576
−0.4951	0.399418	0.47362	0.211832	0.190319
0.405007	0.366504	0.227141	−0.45605	−0.04825
0.317021	0.247876	0.178188	−0.22209	−0.36953
0.468655	0.453673	0.312219	0.09367	−0.27626
0.439435	0.479622	0.152766	0.104102	0.170235
0.10754	−0.06584	0.18084	−0.18537	0.258672
0.32443	0.010942	0.254459	−0.16715	0.162278
0.204052	−0.21247	0.096201	−0.42395	0.20005
0.184792	−0.36655	−0.10054	0.340144	0.344018
0.344462	−0.25382	0.040961	0.066635	0.215148

$$\zeta'_{ij} = \frac{\zeta_{ij} - \zeta_i}{s}$$

$$\bar{\zeta}_i = \frac{1}{m}\sum_{j=1}^{m}\zeta_{ij} \tag{8}$$

$$s_i = \frac{1}{m-1}\sqrt{\sum_{j=1}^{m}(\zeta_{ij} - \bar{\zeta}_i)^2}$$

The ζ'_{ij} values are used for the test of classification capabilities.

Computation SPSS™ version 11.5J was used for the PCA, CATPCA, and MDS calculations. The HNN and ICA calculations were carried out using Fortran programs which we developed. Microsoft Excel™ was used for the scatter plots.

Almost all computations were carried out by a Fujitsu S4/7000 Unix workstation at the Genome Research Information Center, Osaka University. Some of the computations were carried out by a Linux workstation with dual AMD Athlon™ MP1800+ CPUs at our laboratory.

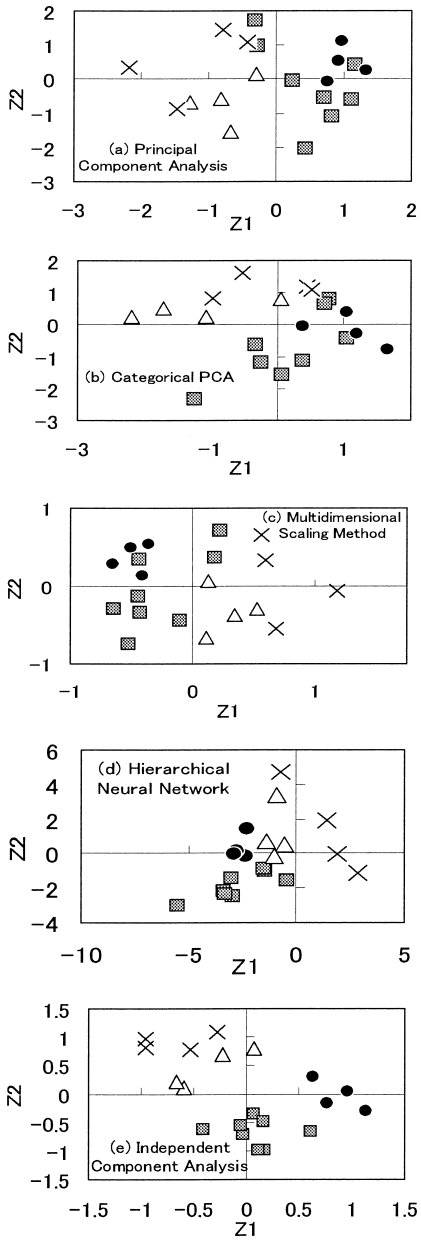

Fig. 2. Two-Dimensional Plots of a Test Data Set (Data-1) Using the Five Classification Methods, (a) PCA, (b) CATPCA, (c) MDS, (d) HNN, and (e) ICA

The four groups are the ones shown in Fig. 1.

Results and Discussion

Artificial Data The five classification methods were applied to the two data sets, which were prepared as stated above. The results are shown in Fig. 2 (Data-1) and Fig. 3 (Data-2). Although, as stated below, ICA showed the best classification results, the results do not directly indicate the classification capability because the four groups had no scientific meanings; that is, it is not necessary to classify the data as in Fig. 1. However, Figures 1—3 show that ICA has the capability to classify data which are difficult to classify using ordinal methods.

PCA (Principal Component Analysis): A correlation coef-

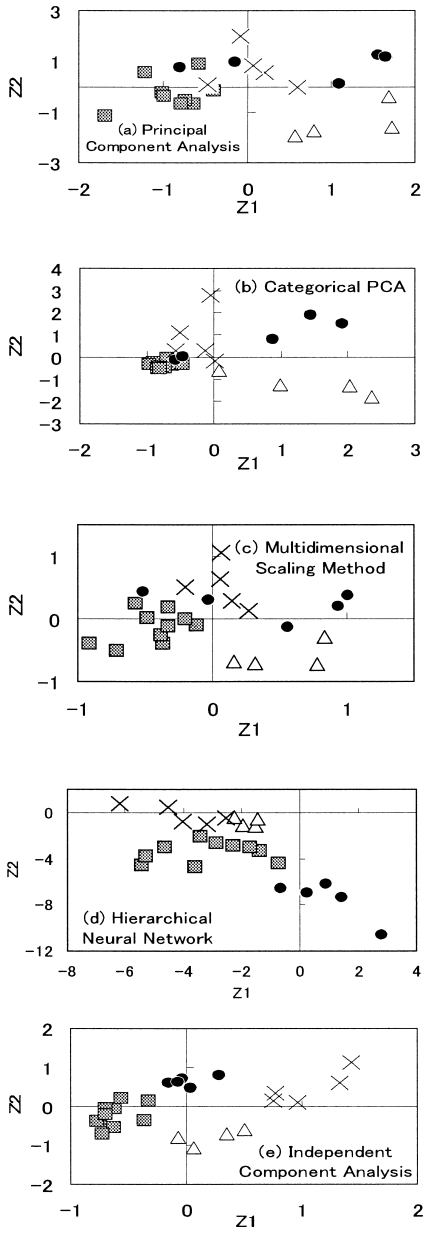

Fig. 3. Two-Dimensional Plots of a Test Data Set (Data-2) Using the Five Classification Methods, Which Are (a) PCA, (b) CATPCA, (c) MDS, (d) HNN, and (e) ICA

The four groups are the ones shown in Fig. 1.

ficients matrix was used for the PCA calculation. The cumulative contribution ratios for the 1st and the 2nd components were 59.40% and 57.31% for Data-1 and Data-2, respectively. In Figs. 2 and 3, scatter plots between the 1st and the 2nd components are shown. Although a 3rd component was also used for the scatter plots, better classification results were not obtained. It is apparent that the PCA method cannot classify the data properly, because the two data sets were prepared so that the PCA is ineffective in the classifying. Thus, although Figs. 2a, 3a show fairly good classification results, they were not adequately classified.

CATPCA (Categorical Principal Component Analysis): CATPCA is a revised method of PCA for categorical data. Initially, the metric data were categorized into 10 categories at even intervals. The categorized data were optimally scaled as second-degree monotonic splines (ordinals) with two interior knots. The cumulative contribution ratios are 69.14% and 73.08%, respectively. Although it was assumed that CATPCA would obtain better classification results than ordinal PCA, CATPCA did not show better scatter plots (Figs. 2b, 3b).

MDS (Multidimensional Scaling Method): Contrary to expectations, MDS showed poor classification capabilities (Figs. 2c, 3c). As stated above, better results were not obtained using other options, such as non-metric methods.

HNN (Hierarchical Neural Networks): Unlike the above three methods, HNN showed fairly good classification capabilities for the data (Figs. 2d, 3d). The number of neurons of the HNN used for the two data sets was 5 (1st and 5th layers), 7 for Data-1 (2nd and 4th layers), 8 for Data-2 (2nd and 4th layers), and 2 (3rd layer). The correlation coefficients between the input and output data were 0.710 (Data-1) and 0.736 (Data-2), respectively. Although better correlation coefficients were obtained when more neurons were used for the 2nd and 4th layers, the resulting scatter plots tended to form a line. Thus, we adopted the HNN with the abovementioned numbers of neurons for each layer.

ICA (Independent Component Analysis): ICA showed the best classification capabilities with regard to the two data sets and the postulated groups shown in Fig. 1. In this study, the learning ratio and inertial force were set to 0.5 and 0.01, respectively. The maximum value of the correlation coefficient between the 1st and 2nd components was set to 0.6. This value was set in order to avoid the scatter plots which tend to form a line. If the correlation coefficient exceeds 0.6, then the neural system stops to learn. The resulting variances of the two components were 0.3607 for the 1st component, 0.4588 for the 2nd component (Data-1), and 0.4500 for the 1st component, 0.3411 for the 2nd component (Data-2). The maximum number of learning times for each iteration was set to 60 in order to avoid overlearning and 20 iterations was carried out. We selected the results of which variances were the maximum as the final results.

Although these results do not directly indicate that ICA can always classify data which is difficult to classify using ordinal methods, it is certain that ICA can be a better tool for classifying and profiling the confiscated drugs. Since ICA can extract the non-normality of data, Hyvarinen and Kano[12] adopted ICA for non-normal factor analysis and succeeded. Thus, it is natural to consider that ICA can be used for classification.

GC-MS Data of Confiscated Methamphetamine The scatter plots of the two components (or axes) obtained by using the five methods are shown in Fig. 4. A correlation coefficients matrix was used for the PCA calculation. The cumulative contribution ratio for the 1st and 2nd components was 15.58%. In the case of CATPCA, the metric data were categorized into 10 categories at even intervals. The categorized data were optimally scaled as second-degree monotonic splines (ordinals) with two interior knots. The cumulative contribution ratio reached 79.01%. When HNN was used, the input data were sphered using PCA; in total, 13 components were used for the input data of the HNN. The self-correlation coefficient of the input data was 0.8424. The maximum value of the correlation ratio between the 1st and 2nd components was set to 0.7. The resulting variances of the two components were 0.3733 and 0.3981 for the 1st and 2nd components,

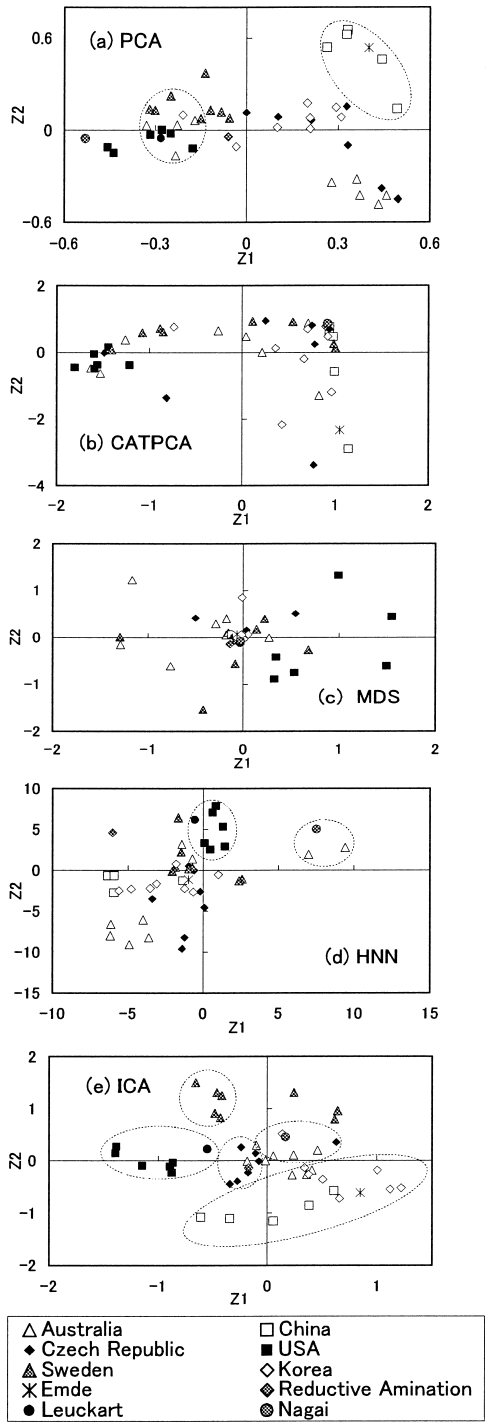

Fig. 4. Classification Results of Confiscated Methamphetamine by the Five Methods, Which Are (a) PCA, (b) CATPCA, (c) MDS, (d) HNN, and (e) ICA

respectively.

Basically, clear-cut classification results do not have to be obtained, even if the best method in the world is used, because samples of methamphetamine confiscated in the same country could have been synthesized by different methods and, in addition, some chemicals such as codeine could have been added. However, it is certain that two methods, CATPCA and MDS, did not succeed in classifying the methamphetamine. When these two methods were used, the four data points of synthesized methamphetamine were in such a small area that no information about the classification or profiling of the confiscated methamphetamine could be obtained. PCA also did not give useful information. On the other hand, because HNN and ICA gave some information about the classification, as shown by the scatter plots of the two methods, we could generally classify the data into several clusters. Especially, ICA showed a more understandable scatter plot than the other four methods. These clusters are shown in Fig. 4 by ellipses with dotted lines. Although these clusters do not contain the same data, some general conclusions can be deduced from the abovementioned ICA results and the chemicals contained in each sample: 1) the methamphetamine confiscated in China could have been synthesized by the Emde method, 2) most of the methamphetamine confiscated in the U.S.A. could have been synthesized by the Leuckard method because it contained *N*-formylmethamphetamine, 1,3-dimethyl-2-phenyl-naphthalene and 1-benzyl-3-methylnaphthalene, which were contained in the synthesized sample by the Leuckard method. 3) some of the methamphetamine confiscated in Australia could have been synthesized by the Nagai method because it did not contain *N*-formylmethamphetamine, which was not contained in the sample synthesized by the Nagai method, but it did contain 1,3-dimethyl-2-phenyl-naphthalene and 1-benzyl-3-methylnaphthalene, which were contained in the samples synthesized by the Nagai method.

From the above results, it can be concluded that this analysis showed that ICA has the capability to be a classification or profiling tool for confiscated methamphetamine.

Table 3. The Summary of This Study

Methods (CCR)[a)]	Artificial Data-1	Artificial Data-2	GC-MS data of confiscated amphethamine
PCA	× (59.40%)	× (57.31%)	△ (15.58%)
CATPCA	× (69.14%)	× (73.08%)	× (79.01%)
MDS	×	×	×
HNN	△	△	△
ICA	○	○	○

a) Cumulative Contribution Ratio. ○: succeeded, △: partly succeeded, ×: not succeeded.

Conclusion

The results of this study are summarized in Table 3. Although this table does not directly indicate that the ICA is the best method for classification, it is certain that the ICA has the capability to classify data which cannot be classified using a normal PCA method.

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