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Technical Report

Comprehensive Detection and Structural Elucidation of Synthetic Cathinones Using GC-MS/MS

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Abstract:

A rapid analytical method that allows comprehensive detection and structural elucidation of synthetic cathinones was developed using a gas chromatograph/tandem mass spectrometer (GC-MS/MS) capable of two-stage mass spectrometry. The proposed method consists of three simultaneous analytical procedures: 1) selective detection of the carbonyl group, characteristic of cathinones, using multiple reaction monitoring (MRM) and determination of both 2) iminium cations and 3) substituted benzoyl cations generated by α-cleavage of amine and benzoyl moieties, respectively, using product ion scan. For all cathinones examined, single peaks were detected at the same retention time on MRM chromatograms in procedure 1) and on total ion current chromatograms (TIC) in procedures 2) and 3). MRM in procedure 1) showed a transition of the substituted benzoyl cation > substituted phenyl cation due to CO elimination by collision-induced dissociation (CID), which demonstrated the existence of a carbonyl group in the structures. Each product ion mass spectrum for the substituted benzoyl cation allowed to not only determine the substituted group on the aromatic ring for all the cathinones, but also differentiate the corresponding positional isomers for ethyl, methoxy, and methylenedioxy substitutions, although identification of the substituted position for methyl, bromine, and fluorine groups on the benzene ring was difficult. On the other hand, the difference in product ion mass spectra between structural isomers of iminium cations was significantly clear, leading to easy discriminative identification of the isomers.

Keywords: synthetic cathinones, designer drugs, GC-MS/MS, structural elucidation

1. Introduction

In recent years, synthetic drugs, whose chemical structures have been partially modified from that of a controlled substance such as a narcotic or stimulant, in order to evade drug regulations, have become a major social problem globally. These include cathinones, which have become the principal drugs involved in synthetic drug abuse, along with indole synthetic cannabinoids. Cathinones (Fig. 1) have a β-keto-phenethyl-amine skeleton and resemble methamphetamine (MA) stimulants in their basic structure, thereby exhibiting a central nervous system-stimulant action similar to that of MA. Various new cathinones are in circulation as synthetic drugs modified with different types of substituents and regioisomers, including modifications to the benzene ring, different types of alkyl groups modifying the α-carbon (so-called side chains), and different types of alkyl groups modifying the nitrogen.

Many methods have been reported for the identification of these synthetic drugs, which mainly involve the use of nuclear magnetic resonance (NMR), gas chromatography/mass spectrometry (GC/MS), or liquid chromatography/tandem mass spectrometry (LC/MS/MS). NMR provides detailed structural information on the constituent hydrogen and carbon atoms of compounds, and is very useful for the structural elucidation. However, it requires several milligrams of isolated and purified objective compounds, making it difficult to apply this approach to highly sensitive analysis of biological samples. Although LC/MS and LC-MS/MS are useful for verifying molecular weight and quantifying drugs in biological samples, they are inferior to GC/MS in terms of retention time precision. Owing to the differences in analysis conditions, LC/MS and LC-MS/MS exhibit differences in the mass spectrum patterns obtained, and thus, are thought to be unsuitable for structural elucidation of unknown cathinones.

Moreover, GC/MS exhibits high retention time precision and allows for simultaneous observation of many ions, reflecting structural differences in the mass spectra obtained through electron ionization (EI). Furthermore, GC/MS shows similar EI mass spectra between instrument types and has many kinds of available spectral databases. Therefore, GC/MS is the most popular method in the field of forensic science.

For the identification of these synthetic drugs, comparison with reference standards is indispensable. However, synthetic drugs that have partially modified chemical structures are not provided as reference standards, and are not registered in mass spectral databases. Thus, there is a high demand for analytical techniques that are applicable, without a reference standard, to structural elucidation and comprehensive detection of cathinones modified with different types of substituents.

Structural elucidation of cathinones is particularly important for determining substituents modifying the benzene ring and hence yielding regioisomers, as well as for certain alkyl group types modifying side chains and the nitrogen and thereby yielding structural isomers. The EI-mass spectra of phenethylamines, obtained using GC/MS, are considered inferior for the detection of structure-reflecting ions, because only a fragment of the α-cleaved amine moiety has relatively high strength.

In this study, we used GC-MS/MS in an EI mode to obtain further cleaved characteristic fragment ions reflective of cathinone substructures. We performed comprehensive detection of cathinones and elucidated their structures, which in turn enabled easy differentiation of cathinone isomers and identification of substituents of various and diverse cathinones.

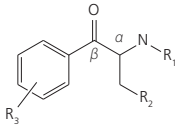

Fig. 1 Main Structure of Cathinones

1 Analytical & Measuring Instruments Division

2. Experimental

A GCMS-TQ8040 triple quadrupole gas chromatograph–mass spectrometer was used for the GC-MS/MS analysis. Table 1 shows detailed analytical conditions. For the evaluation, we selected 62 types of cathinones with different types of substituents located at different positions on the benzene ring and different types of alkyl groups modifying the side chains and nitrogen. Table 2 shows the examined combinations of substituents. As an analysis mode, we performed simultaneous scan/product ion scan/MRM measurements combining three MS/MS measurement types, 1) to 3), in addition to the EI-scan. Fig 2 shows a schematic of this method.

1) MRM measurements accounting for the modification of nine types of substituents to the benzene ring in benzoyl>phenyl transitions
2) Product ion scan measurements using 10 types of different *m/z* produced by *α*-cleavage of the amine as precursor ions
3) Product ion scan measurements using nine types of different *m/z* produced by *α*-cleavage of the benzoyl as precursor ions

In addition, Table 3 shows parameters of MRM and precursor ion scans for ions produced by *α*-cleavage of the benzoyl, and Table 4 shows parameters of precursor ion scans for iminium ions produced by *α*-cleavage of the amine.

Table 1 GC-MS/MS Analytical Conditions

GC/MS	: GCMS-TQ8040
GC conditions	
Column	: SH-Rxi-5Sil MS (length: 30 m, inner diameter: 0.25 mm, film thickness 0.25 µm)
Injection temperature	: 260°C
Column oven temperature	: 60°C (2 min) – (15°C/min) – 320°C (5 min)
Carrier gas	: Helium
Flow control	: Constant linear velocity (45.6 cm/sec)
Injection mode	: Splitless
MS conditions	
Ionization mode	: EI
Ion source temperature	: 200°C
Interface temperature	: 280°C
Analysis mode	: Scan/product ion scan/MRM simultaneous measurement
Collision gas	: Argon (200 kPa)

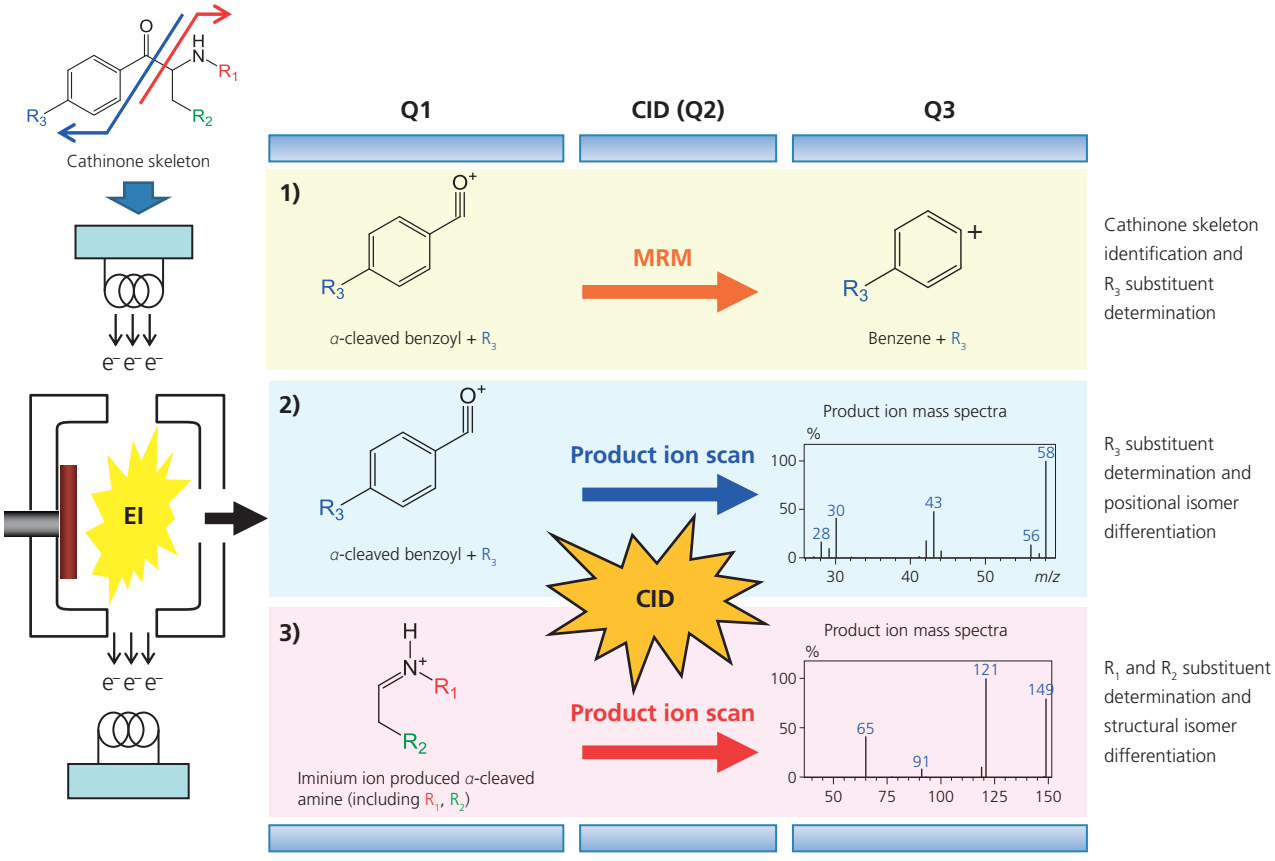

Fig. 2 Schematic of Three Types of MS/MS Measurements

Table 2 Evaluated Cathinones and Their Substituents

No.	Compound	R_1	R_2	R_3
1	Methcathinone	Methyl	H	H
2	*N*-Ethyl-*N*-methylcathinone	*N*-Ethyl-*N*-methyl	H	H
3	Ethcathinone	Ethyl	H	H
4	*N*,*N*-Diethylcathinone	*N*,*N*-Diethyl	H	H
5	α-PPP	Pyrrolidinyl	H	H
6	Buphedrone	Methyl	Methyl	H
7	*N*-Ethyl-*N*-methylbuphedone	*N*-Ethyl-*N*-methyl	Methyl	H
8	*N*-Ethylbuphedrone (NEB)	Ethyl	Methyl	H
9	*N*,*N*-Diethylbuphedrone	*N*,*N*-Diethyl	Methyl	H
10	α-PBP	Pyrrolidinyl	Methyl	H
11	Pentedrone	Methyl	Ethyl	H
12	*N*-Ethyl-*N*-methylpentedrone	*N*-Ethyl-*N*-methyl	Ethyl	H
13	*N*-Ethylpentedrone	Ethyl	Ethyl	H
14	*N*,*N*-Diethylpentedrone	*N*,*N*-Diethyl	Ethyl	H
15	α-PVP	Pyrrolidinyl	Ethyl	H
16	*N*-Desmethylhexedrone	H	*n*-Propyl	H
17	Hexedrone	Methyl	*n*-Propyl	H
18	*N*,*N*-Dimethylhexedrone	*N*,*N*-Dimethyl	*n*-Propyl	H
19	α-PHP	Pyrrolidinyl	*n*-Propyl	H
20	α-PHPP	Pyrrolidinyl	*n*-Butyl	H
21	α-POP	Pyrrolidinyl	*n*-Pentyl	H
22	α-PNP	Pyrrolidinyl	*n*-Hexyl	H
23	2-Methylmethcathinone	Methyl	H	Methyl (*ortho*)
24	3-Methylmethcathinone	Methyl	H	Methyl (*meta*)
25	4-Methylmethcathinone	Methyl	H	Methyl (*para*)
26	4-Methylethcathinone	Ethyl	H	Methyl (*para*)
27	MPPP (Desethylpyrovalerone)	Pyrrolidinyl	H	Methyl (*para*)
28	4-Methylbuphedrone	Methyl	Methyl	Methyl (*para*)
29	4-Methyl-*N*-ethylbuphedrone	Ethyl	Methyl	Methyl (*para*)
30	MPBP	Pyrrolidinyl	Methyl	Methyl (*para*)
31	4-Methylpentedrone	Methyl	Ethyl	Methyl (*para*)
32	4-Ethyl-*N*-ethylpentedrone	Ethyl	Ethyl	Ethyl (*para*)
33	MPVP	Pyrrolidinyl	Ethyl	Methyl (*para*)
34	4-Ethylcathinone	H	H	Ethyl (*para*)
35	2-Ethylmethcathinone	Methyl	H	Ethyl (*ortho*)
36	3-Ethylmethcathinone	Methyl	H	Ethyl (*meta*)
37	4-Ethylmethcathinone	Methyl	H	Ethyl (*para*)
38	4-Ethyl-*N*,*N*-dimethylcathinone	*N*,*N*-Dimethyl	H	Ethyl (*para*)
39	2-Bromomethcathinone	Methyl	H	Br (*ortho*)
40	3-Bromomethcathinone	Methyl	H	Br (*meta*)
41	4-Bromomethcathinone	Methyl	H	Br (*para*)
42	4-Chloromethcathinone	Methyl	H	Cl (*para*)
43	2-Fluoromethcathinone	Methyl	H	F (*ortho*)
44	3-Fluoromethcathinone	Methyl	H	F (*meta*)
45	4-Fluoromethcathinone	Methyl	H	F (*para*)
46	4-Fluorooctedrone (4F-Octedrone)	Methyl	*n*-Pentyl	F (*para*)
47	4-Iodomethcathinone	Methyl	H	I (*para*)
48	2-Methoxymethcathinone	Methyl	H	Methoxy (*ortho*)
49	3-Methoxymethcathinone	Methyl	H	Methoxy (*meta*)
50	4-Methoxymethcathinone	Methyl	H	Methoxy (*para*)
51	4-Methoxyethcathinone	Ethyl	H	Methoxy (*para*)
52	MOPPP	Pyrrolidinyl	H	Methoxy (*para*)
53	2,3-Methylenedioxymethcathinone	Methyl	H	Methylnedioxy (2,3-)
54	Methylone (bk-MDMA)	Methyl	H	Methylnedioxy (3,4-)
55	Ethylone (bk-MDEA)	Ethyl	H	Methylnedioxy (3,4-)
56	MDPPP	Pyrrolidinyl	H	Methylnedioxy (3,4-)
57	bk-BDB	H	Methyl	Methylnedioxy (3,4-)
58	bk-MBDB	Methyl	Methyl	Methylnedioxy (3,4-)
59	3,4-Methylenedioxy-*N*,*N*-dimethylbuphedrone	*N*,*N*-Dimethyl	Methyl	Methylnedioxy (3,4-)
60	Buthylone	H	Ethyl	Methylnedioxy (3,4-)
61	Penthylone	Methyl	Ethyl	Methylnedioxy (3,4-)
62	*N*,*N*-Dimethylpentylone	*N*,*N*-Dimethyl	Ethyl	Methylnedioxy (3,4-)

Table 3 MRM Transition and Precursor *m/z* of a Product Ion Scan for the α-Cleaved Benzoyl

Precursor *m/z*	MRM transition	R_3	CE (V)
105	105 > 77	H	10
119	119 > 91	Methyl	10
123	123 > 95	F	10
133	133 > 105	Ethyl or Dimethyl	10
135	135 > 107	Methoxy	10
139	139 > 111	Cl	10
149	149 > 121	Methylenedioxy	10
183	183 > 155	Br	10
231	231 > 203	I	10

Table 4 Precursor *m/z* of a Product Ion Scan for Iminium Ions Produced by α-Cleaved Amine

Precursor *m/z*	R_1	R_2	CE (V)
44	H	H	15
58	Methyl	H	15
	H	Methyl	
72	*N*,*N*-Dimethyl	H	15
	Ethyl	H	
	Methyl	Methyl	
	H	Ethyl	
86	*N*-Ethyl-*N*-methyl	H	15
	N,*N*-Dimethyl	Methyl	
	Ethyl	Methyl	
	Methyl	Ethyl	
	H	*n*-Propyl	
98	Pyrrolidinyl	H	15
100	*N*,*N*-Diethyl	H	15
	N-Ethyl-*N*-methyl	Methyl	
	N,*N*-Dimethyl	Ethyl	
	Ethyl	Ethyl	
	Methyl	*n*-Propyl	
	H	*n*-Butyl	
112	Pyrrolidinyl	CH_3	15
114	*N*,*N*-Diethyl	Methyl	15
	N-Ethyl-*N*-methyl	Ethyl	
	N,*N*-Dimethyl	*n*-Propyl	
	Ethyl	*n*-Propyl	
	Methyl	*n*-Butyl	
	H	*n*-Pentyl	
126	Pyrrolidinyl	Ethyl	15

Precursor *m/z*	R_1	R_2	CE (V)
128	*N*,*N*-Diethyl	Ethyl	15
	N-Ethyl-*N*-methyl	*n*-Propyl	
	N,*N*-Dimethyl	*n*-Butyl	
	Ethyl	*n*-Butyl	
	Methyl	*n*-Pentyl	
	H	*n*-Hexyl	
140	Pyrrolidinyl	*n*-Propyl	15
142	*N*,*N*-Diethyl	*n*-Propyl	15
	N-Ethyl-*N*-methyl	*n*-Butyl	
	N,*N*-Dimethyl	*n*-Pentyl	
	Ethyl	*n*-Pentyl	
	Methyl	*n*-Hexyl	
	H	*n*-Heptyl	
154	Pyrrolidinyl	*n*-Butyl	15
156	*N*,*N*-Diethyl	*n*-Butyl	15
	N-Ethyl-*N*-methyl	*n*-Pentyl	
	N,*N*-Dimethyl	*n*-Hexyl	
	Ethyl	*n*-Hexyl	
	Methyl	*n*-Heptyl	
168	Pyrrolidinyl	*n*-Pentyl	15
170	*N*,*N*-Diethyl	*n*-Pentyl	15
	N-Ethyl-*N*-methyl	*n*-Hexyl	
	N,*N*-Dimethyl	*n*-Heptyl	
	Ethyl	*n*-Heptyl	
182	Pyrrolidinyl	*n*-Hexyl	15
184	*N*,*N*-Diethyl	*n*-Hexyl	15
	N-Ethyl-*N*-methyl	*n*-Heptyl	
196	Pyrrolidinyl	*n*-Heptyl	15
198	*N*,*N*-Diethyl	*n*-Heptyl	15

3. Results and Discussion

3-1. Detection of Benzoyl Skeletons by MRM Measurement

It is known that benzoyl cations produced by α-cleavage of the benzoyl and ions eliminated with a CO molecule from benzoyl cations are observed in EI-mass spectra of cathinones. These ions have a weak relative intensity compared to the iminium ion produced by α-cleavage of the amine. However, the presence of β-carbonyl groups is very important for the differentiation of cathinones and phenethylamines. Therefore, we attempted to selectively detect cathinones with the carbonyl group using the MRM transition of the benzyl cation as a precursor ion and benzene as a product ion, with carbonyl eliminated by collision-induced dissociation (CID). We set MRM transitions corresponding to combinations of "benzoyl>phenyl" accounting for the masses of nine types of substituents modifying the benzene ring.

We evaluated the optimal CID collision energy in as many established MRM measurements as possible and set the collision energy for all MRM measurements at 10 V. In addition, MRM transitions corresponding to combinations of "benzoyl>phenyl" were verified in all 62 types of cathinones examined.

Identification of cathinones requires the verification of two types of ions present in EI-mass spectra, benzoyl cations produced by α-cleavage of the benzoyl and ions eliminated with the CO molecule from benzoyl cations. However, relative intensities of these ions are very weak with EI-scans, making data processing of mass spectra time-consuming. In addition, sometimes these ions are buried in the background noise of biological samples or low-concentration samples, which increases the risk of misidentification.

Since CO elimination from benzoyl cations was selectively monitored in MRM measurements, it was possible to detect the presence of two types of ions produced from this reaction as peaks on MRM chromatograms. Therefore, it was easy to detect the benzoyl skeleton, characteristic of cathinones. In addition, when a peak of set MRM transitions corresponding to substituents modifying benzene rings was detected, the types of substituents modifying the benzene ring could be identified.

3-2. Product Ion Scan Measurement of Ions Produced by α-Cleavage of Benzoyl

If a MRM measurement in section 3-1 suggested the possibility of a cathinone, further specification, such as a modified position of substituents to the benzene ring, was important for structure elucidation. Therefore, we utilized a product ion scan, which accounts for the substituents shown in Table 3, to determine both positions and types of substituents attached to the benzene ring. Regarding the compounds examined, in addition to the basic methcathinone skeleton, methyl groups, ethyl groups, methoxy groups, methylenedioxy groups, bromine, and fluorine as substituents modifying the benzene ring and their *o*-, *m*-, and *p*-position substituents for regioisomers were selected.

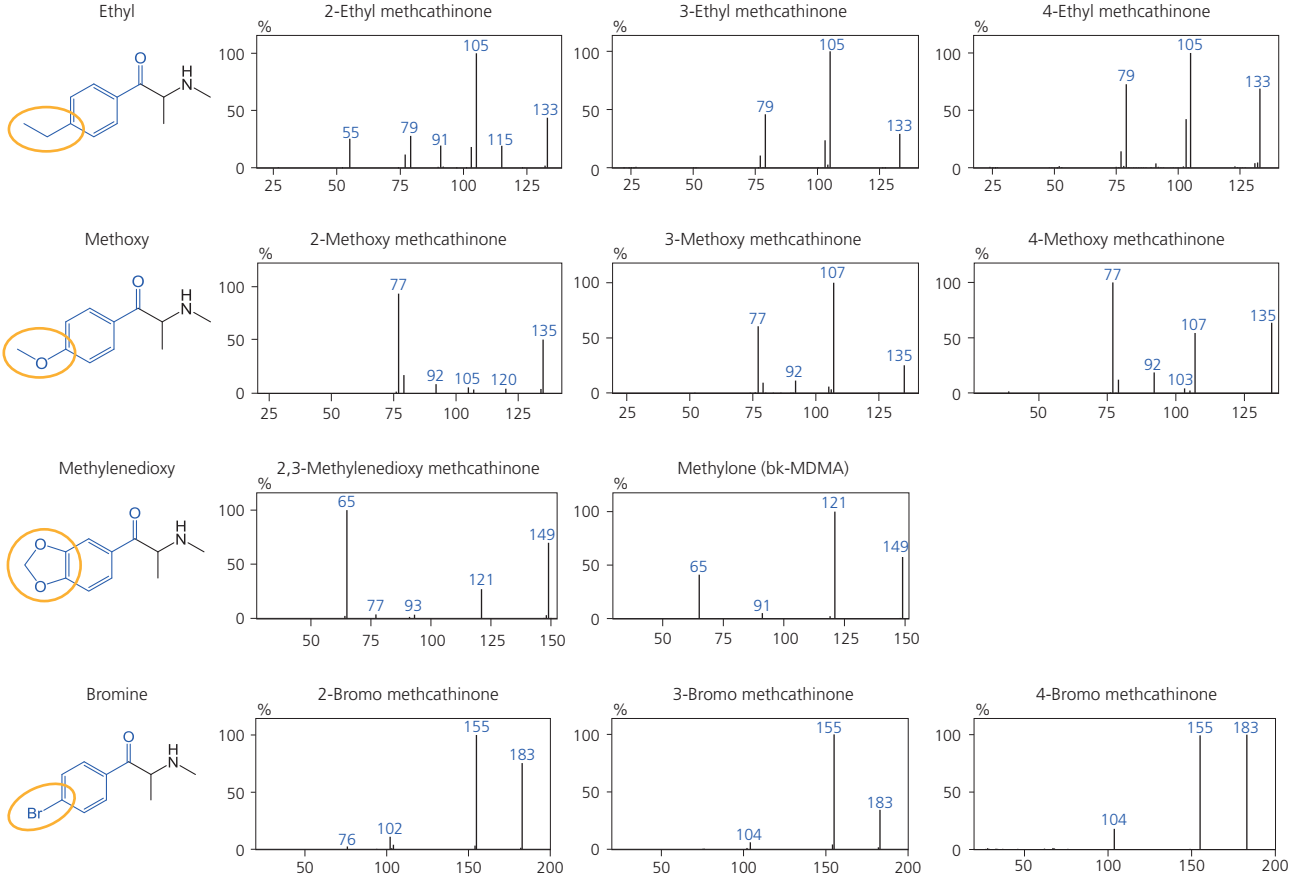

Fig. 3 Product Ion Mass Spectra of α-Cleaved Benzoyl Cations

For each compound, we set benzoyl cations produced by α-cleavage of benzoyl as precursor *m/z* and optimized the CID collision energy to obtain product ion mass spectra changing the collision energy. In the case when a methyl or ethyl group was substituted to the benzene ring, if the collision energy was set higher, elimination of methyl or ethyl group substituted to the benzene ring occurred, and the ion intensity reflecting the structure of the aromatic ring side chain was relatively weak. Therefore, the optimal collision energy was set at 10 V. Fig. 3 shows representative product ion mass spectra.

If an ethyl, methoxy, or methylenedioxy group was substituted to the benzene ring, three or more characteristic ions with a high relative intensity were observed in each product ion spectrum.

In addition, their regioisomers could be differentiated by the relative intensity and respective characteristic ions. However, if a methyl, bromine, or fluorine group was substituted to the benzene ring, only two types of ions were observed, a precursor ion and an ion eliminated with the CO molecule from each precursor ion. In the case of these substituents, it was possible to identify the type of the substituent, but regioisomers were difficult to differentiate from the product ion in a mass spectrum.

3-3. Product Ion Scan Measurement of Ions Produced by α-Cleavage of the Amine

It is known that iminium ions derived from α-cleavage of the amine are detected with a high intensity in EI-mass spectra of cathinones. Amine skeletons forming iminium ions produced by α-cleavage of the amine have many structural isomers. However, identifying structural isomers of the amine moiety is difficult using only EI-mass spectra. Therefore, we attempted to elucidate amine moieties using the mass spectrum of a product ion scan, with iminium ions produced by the α-cleaved amine set as precursor *m/z*.

Product ion mass spectra are largely dependent on the collision energy. Therefore, we examined the optimum collision energy allowing for structural isomer differentiation of amine moieties. We determined that 15 eV was the optimum collision energy, at which product ions reflecting differences in the amine moiety were observed with a relatively strong intensity in the product ion mass spectra.

Representative product ion mass spectra obtained using iminium ions produced by α-cleavage of the amine as precursor ions are shown in Fig. 4 (precursor *m/z* 86) and Fig. 5 (precursor *m/z* 100). The mass spectrum patterns were clearly different even if precursor ions of the same *m/z* were selected. These differences were reflective of the amine grade and the type of the alkyl group substituted to the nitrogen atom, and were evidenced by different base peak *m/z*, allowing for easy differentiation of structural isomers.

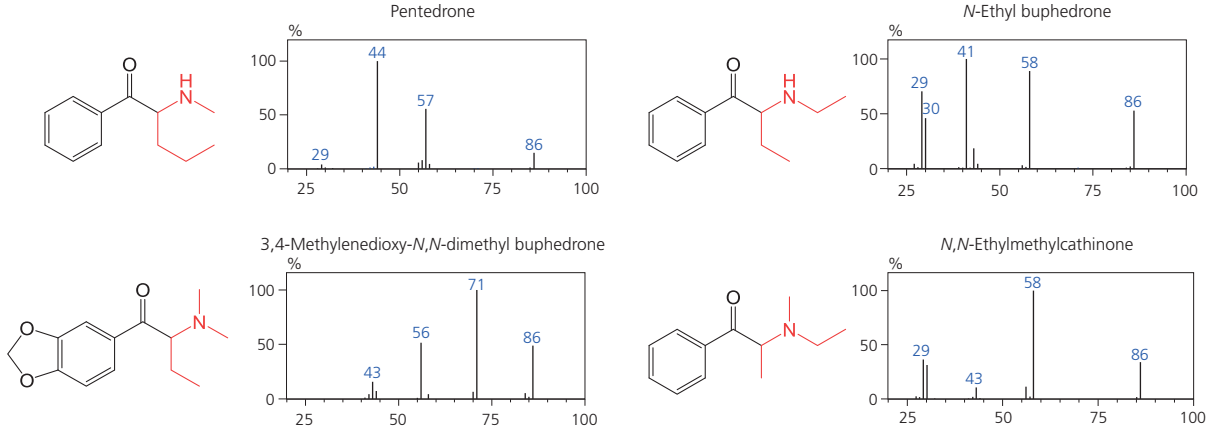

Fig. 4 Product Ion Mass Spectra Using Iminium Ion *m/z* 86 Produced by α-Cleavage of the Amine

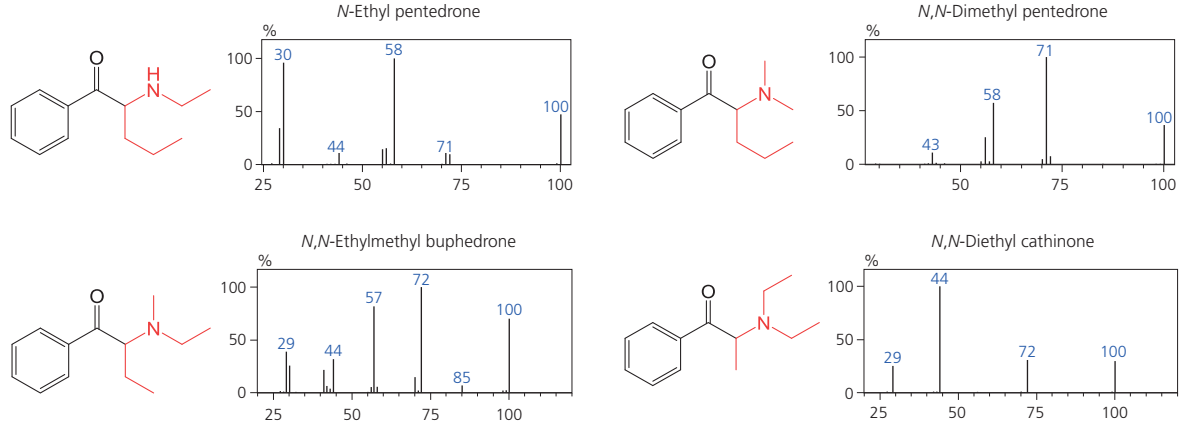

Fig. 5 Product Ion Mass Spectra Using Iminium Ion *m/z* 100 Produced by α-Cleavage of the Amine

3-4. Example of Comprehensive Detection and Structural Elucidation Using This Technique

Combining the three types of MS/MS measurements in theory enables the comprehensive detection and structural elucidation of cathinones. If a sample containing cathinone is analyzed, peaks on chromatograms obtained from the three respective types of MS/MS measurements are detected at the same retention times. By confirming the transitions observed in the MRM chromatogram peak, it is possible to evaluate whether the detected peak has the characteristic cathinone structure and which of the nine substituents modifies the benzene ring.

In addition, based on the results from product ion scan measurements of ions produced by α-cleavage of the benzoyl group, it is possible to determine substituents modifying the benzene ring by automatically searching pre-registered product ion spectrum databases for product ion spectra. Moreover, the positional isomer can be specified according to the type of substituents. In addition, based on the results from the product ion scan, in which iminium ions produced by α-cleavage of the amine are used as precursors, amine moieties can be identified.

Fig. 6 shows an example of the analysis performed using this method. A cathinone was detected, and three chromatograms from each MS/MS measurement type were obtained with the same retention times in each respective measurement. The MRM transition (*m/z* 133>105) of the obtained MRM chromatogram (1) confirmed that the peak had a characteristic cathinone structure, and the substituent modifying the benzene ring was a dimethyl or ethyl group.

In addition, the product ion spectra of precursor *m/z* 133 produced by α-cleavage of the benzoyl as precursors indicated that an ethyl group modified the *m*-position (2). Furthermore, the result of the product ion scan of *m/z* 58 produced by α-cleavage of the amine indicated that the amine moiety consisted of $R_1 = CH_3$, R_2 :H (3). Based on these results, the detected peak was estimated to be 3-ethylmethcathinone. Measurement of a reference standard showed an identical retention time, confirming the detected peak as 3-ethylmethcathinone.

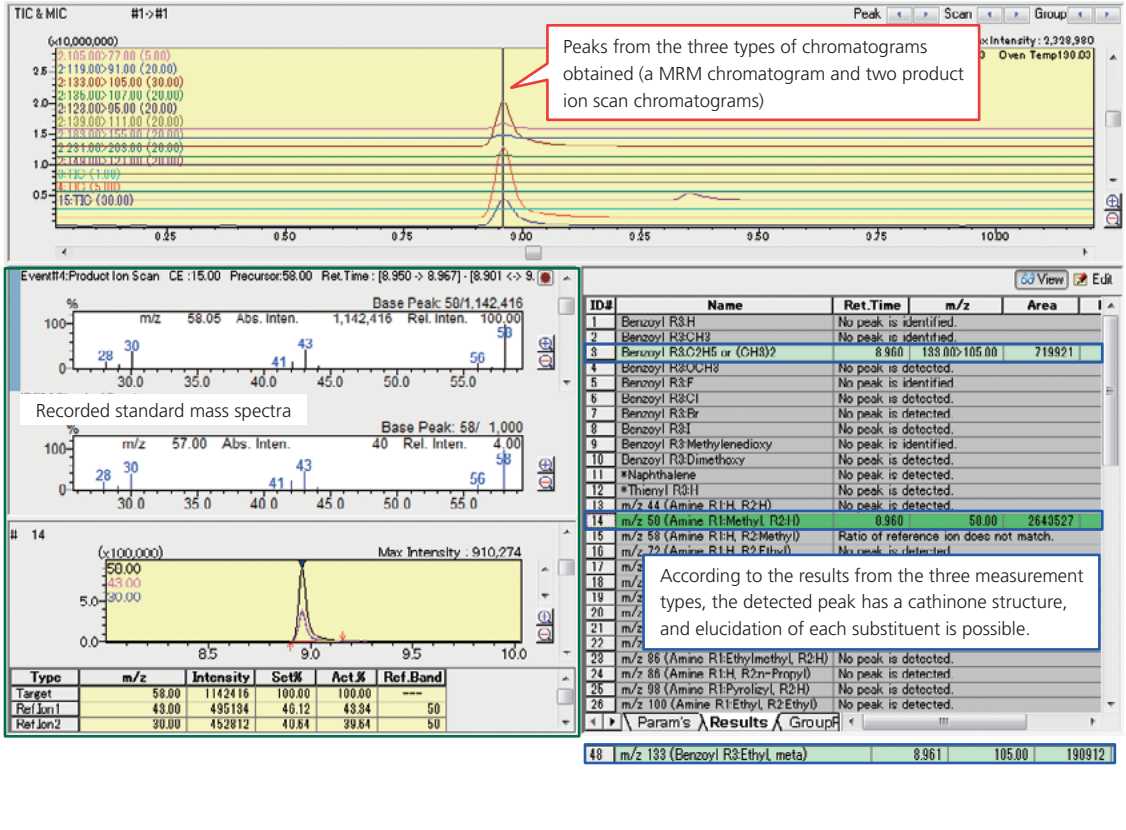

Fig. 6 Data Processing Procedures Using This Proposed Method

4. Conclusions

We performed comprehensive detection and structural elucidation of cathinones using MRM and product ion scans with GC-MS/MS. By combining measurements from product ion scans, which use precursor ions reflective of the structure of the α-cleaved amine and benzoyl produced by EI, and MRM, which selectively detects the benzoyl moiety, all examined cathinones could be detected on individual MRM chromatograms.

In product ion scans using iminium ions produced by α-cleavage of the amine as precursors, clear differences were observed for base peaks in the product ion spectra, as well as in the mass spectral pattern. The product ion scan allows elucidation of the substructure of the amine moiety, which is difficult to achieve using an EI-scan with GC/MS. In product ion measurements using ions produced by α-cleavage of the benzoyl as precursors, it was difficult to distinguish the regioisomers of some substituents, such as methyl group and halogen atoms. However, the regioisomers of ethyl, methoxy, and methylenedioxy groups could be differentiated by the mass spectral pattern.

GC-MS/MS allows ions fragmented by EI to be cleaved by CID. The main structure of cathinones is divided into two substructures, amine and benzoyl moieties, which are analyzed independently for the structural elucidation. A collection of product ion mass spectra of amine and benzoyl substructures can greatly reduce the effort required to obtain reference standards for comparison with the collection of EI-scan mass spectra of each individual cathinone. In recent years, new synthetic cathinones have been circulated, such as α-PVT modified with a thienyl group instead of the benzoyl moiety. Cathinones with partial structural modifications are expected to widely circulate in the future. A collection of additional information on MRM transitions and product ion scan mass spectra reflecting these substructures is expected to be very useful for the structural elucidation of newly derived cathinones.

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- Capable of performing high-sensitivity analysis even as a single GC-MS system.

Simultaneous measurement in a multiple analysis mode

GCMS-TQ8040 achieved a maximum scanning speed of 20,000 u/sec using a high-efficiency collision cell UF sweeper, which is capable of achieving a high CID efficiency and high-speed ion transport with Advanced Scanning Speed Protocol (ASSP). Using this application, a three-mode simultaneous measurement (scan/MRM/product ion scan) is performed. It is possible to use product ion scanning with a maximum scanning speed of 20,000 u/sec, allowing for 10 or more precursor *m/z* types per single run.

	Compound Name	Start Time (min)	End Time (min)	Acq. Mode	Event Time(sec)	Scan Speed	Start m/z	End m/z	Precursor m/z	CE
1-1		2.30	43.00	Q3 Scan	0.050	10000	43.00	500.00		
1-2		2.30	43.00	MRM	0.050					
1-3	Amine m/z44	2.30	43.00	Product Ion Scan	0.005	20000	20.00	45.00	44.00	15.00
1-4	Amine m/z58	2.30	43.00	Product Ion Scan	0.005	20000	20.00	59.00	58.00	15.00
1-5	Amine m/z72	2.30	43.00	Product Ion Scan	0.008	20000	20.00	73.00	72.00	15.00
1-6	Amine m/z86	2.30	43.00	Product Ion Scan	0.008	20000	20.00	87.00	86.00	15.00
1-7	Amine m/z98	2.30	43.00	Product Ion Scan	0.010	20000	20.00	99.00	98.00	15.00
1-8	Amine m/z100	2.30	43.00	Product Ion Scan	0.010	20000	20.00	101.00	100.00	15.00
1-9	Amine m/z112	2.30	43.00	Product Ion Scan	0.010	20000	20.00	113.00	112.00	15.00
1-10	Amine m/z114	2.30	43.00	Product Ion Scan	0.010	20000	20.00	115.00	114.00	15.00
1-11	Amine m/z126	2.30	43.00	Product Ion Scan	0.010	20000	20.00	127.00	126.00	15.00
1-12	Amine m/z128	2.30	43.00	Product Ion Scan	0.010	20000	20.00	129.00	128.00	15.00
1-13	Amine m/z140	2.30	43.00	Product Ion Scan	0.010	20000	20.00	141.00	140.00	15.00
1-14	Amine m/z142	2.30	43.00	Product Ion Scan	0.015	20000	20.00	143.00	142.00	15.00
1-15	Amine m/z154	2.30	43.00	Product Ion Scan	0.015	20000	20.00	155.00	154.00	15.00
1-16	Amine m/z156	2.30	43.00	Product Ion Scan	0.015	20000	20.00	157.00	156.00	15.00
1-17	Amine m/z168	2.30	43.00	Product Ion Scan	0.015	20000	20.00	169.00	168.00	15.00
1-18	Amine m/z170	2.30	43.00	Product Ion Scan	0.015	20000	20.00	171.00	170.00	15.00
1-19	Amine m/z182	2.30	43.00	Product Ion Scan	0.015	20000	20.00	183.00	182.00	15.00
1-20	Amine m/z184	2.30	43.00	Product Ion Scan	0.015	20000	20.00	185.00	184.00	15.00
1-21	Amine m/z196	2.30	43.00	Product Ion Scan	0.015	20000	20.00	197.00	196.00	15.00
1-22	Amine m/z198	2.30	43.00	Product Ion Scan	0.015	20000	20.00	199.00	198.00	15.00
1-23	Benzoyl R3:H	2.30	43.00	Product Ion Scan	0.012	10000	20.00	106.00	105.00	10.00
1-24	Benzoyl R3:Methyl	2.30	43.00	Product Ion Scan	0.015	10000	20.00	120.00	119.00	10.00
1-25	Benzoyl R3:Ethyl or Dimet	2.30	43.00	Product Ion Scan	0.015	10000	20.00	134.00	133.00	10.00
1-26	Benzoyl R3:Methoxy	2.30	43.00	Product Ion Scan	0.015	10000	20.00	136.00	135.00	10.00
1-27	Benzoyl R3:F	2.30	43.00	Product Ion Scan	0.015	10000	20.00	124.00	123.00	10.00
1-28	Benzoyl R3:Cl	2.30	43.00	Product Ion Scan	0.015	10000	20.00	140.00	139.00	10.00
1-29	Benzoyl R3:Br	2.30	43.00	Product Ion Scan	0.020	10000	20.00	184.00	183.00	10.00
1-30	Benzoyl R3:I	2.30	43.00	Product Ion Scan	0.025	10000	20.00	232.00	231.00	10.00
1-31	Benzoyl R3:Methylenediox	2.30	43.00	Product Ion Scan	0.020	10000	20.00	150.00	149.00	10.00
1-32	Thienyl R3:H	2.30	43.00	Product Ion Scan	0.012	10000	20.00	112.00	111.00	10.00
1-33	Benzoyl R3:Dimethoxy	2.30	43.00	Product Ion Scan	0.020	10000	20.00	166.00	165.00	10.00
1-34	Naphthalene R3:H	2.30	43.00	Product Ion Scan	0.020	10000	20.00	156.00	155.00	10.00

MS/MS analysis conditions in this application

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