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Characterization of the designer drug deschloroketamine (2-methylamino-2-phenylcyclohexanone) by gas chromatography/mass spectrometry, liquid chromatography/high-resolution mass spectrometry, multistage mass spectrometry, and nuclear magnetic resonance

Giampietro Frison[1]*, Luca Zamengo[1], Flavio Zancanaro[1], Francesco Tisato[2] and Pietro Traldi[2]

[1]Laboratory of Environmental Hygiene and Forensic Toxicology, Department of Prevention, Azienda ULSS 12, Veneziana, Italy
[2]IENI – CNR, Corso Stati Uniti 4 35127 Padova, Italy

RATIONALE: Clinical and forensic toxicology laboratories are challenged every day by the analytical aspects of the new psychoactive substances phenomenon. In this study we describe the analytical characterization of a new ketamine derivative, deschloroketamine (2-methylamino-2-phenylcyclohexanone), contained in seized powders.
METHODS: The analytical techniques employed include gas chromatography/mass spectrometry (GC/MS), liquid chromatography/electrospray ionization coupled with Orbitrap high-resolution/MS (LC/ESI-HRMS), multistage MS (ESI-MS^n), and NMR. The LC/ESI-HRMS analyses consisted of accurate mass measurements of MH^+ ions in full-scan mode; comparison of experimental and calculated MH^+ isotopic patterns; and examination of the isotopic fine structure (IFS) of the M + 1, M + 2, M + 3 isotopic peaks relative to the monoisotopic M + 0 peak. The collision-induced product ions of the MH^+ ions were studied by both HRMS and MS^n. ^1H and ^{13}C NMR measurements were carried out to confirm the chemical structure of the analyte.
RESULTS: The EI mass spectra obtained by GC/MS analysis showed the presence of molecular ions at *m/z* 203, and main fragment ions at *m/z* 175, 174, 160, 147, 146, and 132. The application of LC/ESI-HRMS allowed us to obtain: the accurate mass of deschloroketamine MH^+ ions with a mass accuracy of 1.47 ppm; fully superimposable experimental and calculated MH^+ isotopic patterns, with a relative isotopic abundance value of 3.69 %; and the IFS of the M + 1, M + 2, M + 3 isotopic peaks completely in accordance with theoretical values. Examination of the product ions of MH^+, as well as the study of both ^1H and ^{13}C NMR spectra, enabled the full characterization of the molecular structure of deschloroketamine.
CONCLUSIONS: The combination of the employed analytical techniques allowed the characterization of the seized psychoactive substance, in spite of the lack of a reference standard. Deschloroketamine is a ketamine analogue considered to be more potent and longer lasting than ketamine, and this paper is probably the first to report on its analytical characterization. Copyright © 2015 John Wiley & Sons, Ltd.

The growth in the production of new psychoactive substances (NPS) is a complex phenomenon that affects both the health and the security of citizens worldwide. Amphetamine-related designer drugs (mainly phenethylamines, tryptamines, piperazines and cathinones), as well as synthetic cannabinoids, are the NPS that most frequently appear on the recreational drug market. According to the European Monitoring Centre for Drugs and Drug Addiction (EMCDDA) 2015 Update on NPS in Europe,[1] there has been a seven-fold increase in reported seizures of NPS between 2008 and 2013, and more than 450 NPS are currently being monitored by the EMCDDA. In addition, according to the United Nations Office on Drugs and Crime (UNODC) 2014 World Drug Report,[2] the number of NPS on the global drug market clearly exceeds the number of traditional psychoactive substances controlled at the international level. Moreover, the risks associated with the use of NPS, due to the high variability of concentration of active ingredients, mislabelled preparations, and multiple NPS in single products, are a source of concern for possible serious health-related consequences, particularly for young people.[3]

Clinical and forensic toxicology laboratories are required to identify, sometimes very quickly, NPS in both seized materials and biological fluids, often without the availability of reference standards or analytical data from the scientific literature. The Scientific Working Group for the Analysis of

* *Correspondence to:* G. Frison, Laboratory of Environmental Hygiene and Forensic Toxicology, Department of Prevention, Azienda ULSS 12, Veneziana, Italy.
E-mail: giampietro.frison@ulss12.ve.it

Seized Drugs (SWGDRUG) recommendations suggest the use of multiple uncorrelated analytical techniques for the forensic identification of a seized drug.[4] This approach is particularly important for the identification of a new drug in the absence of a reference material, as also underlined by UNODC in a report on the challenge of NPS.[5] Thus, the combination of results obtained from the application of mass spectrometry (MS) techniques, such as tandem MS (MS/MS) and high-resolution MS (HRMS), with those obtained from nuclear magnetic resonance (NMR) and/or infrared (IR) spectroscopy, can help in elucidating the structures of unknown substances, in the absence of reference materials or without resorting to the synthesis of *ad hoc* standards. We recently adopted this approach for the analytical characterization of the designer drug bk-2C-B contained in a seized tablet.[6]

In addition to amphetamine-related NPS and synthetic cannabinoids, in recent years some new analogs of ketamine have entered the illegal drugs market. Ketamine (2-(2-chlorophenyl)-2-(methylamino)cyclohexanone) (Fig. 1(a)) is a NMDA-receptor-antagonist used as an anaesthetic in both human and veterinary medicine. It causes depression of the central nervous system, resulting in hallucinations, and disturbances in thinking, perception, and motor function. Ketamine is also even used for recreational purposes, following its illicit synthesis or utilizing preparations diverted from the pharmaceutical supply to hospitals.[7] Among the new ketamine analogs, one of the most abused is methoxetamine (2-(ethylamino)-2-(3-methoxyphenyl)cyclohexanone) (Fig.1(b)), which produces a dissociative catatonic state in users similar to that seen with ketamine, accompanied by sympathomimetic toxicity, with significant tachycardia and hypertension.[8,9] Furthermore, the lycaeum.org/rhodium Internet site mentions that another ketamine analog has been found on the black market: a compound missing the 2-chloro substituent on the ketamine phenyl ring.[10] According to the same site, this compound is considered to be more potent and longer lasting than ketamine. At the time of writing there are few Internet references to this designer drug: the alert released on March 26, 2015, on the website of Energy Control, a Spanish non-governmental organization (NGO) with the aim of risk reduction, providing information and analysis of street drugs,[11] and the users forum on the Chemsrus website.[12] However, to the best of our knowledge, no reports on the analytical characterization of this designer drug have been published or appeared on the Internet.

Within the framework of our forensic toxicology activities we were recently asked to analyze several off-white powders seized by police. The powders were contained in 102 envelopes of three different colours (31 green, 20 pink and 51 blue), all made of square pieces of paper folded in the way typically used for selling ketamine-containing powders on the recreational market. Although the drug dealer claimed that all the powders should have contained ketamine, methoxetamine was identified in the powders contained in the pink envelopes, while a ketamine derivative, which we named deschloroketamine (2-methylamino-2-phenylcyclohexanone; Fig. 1(c)) as it has exactly the same structure as ketamine although without the chlorine substituent on the phenyl ring, was identified in the powders contained in the green and blue envelopes. This represents, to the best of our knowledge, the first seizure of deschloroketamine in Italy, and this paper is probably the first to report on its analytical characterization.

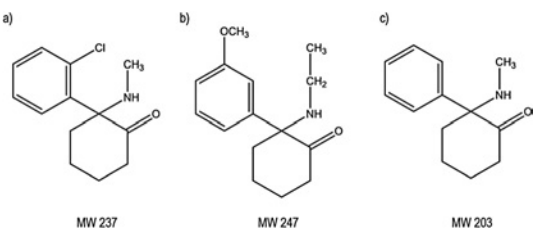

Figure 1. Chemical structures and molecular weights of (a) ketamine, (b) methoxetamine, and (c) deschloroketamine.

In this study we describe the analytical approach adopted for the characterization of the deschloroketamine. In addition to the lack of reports on its identification, no certified analytical standard is commercially available. Moreover, because of the need to obtain prompt characterization of the drug for the police, synthesis of the deschloroketamine for comparison purposes was not possible. The analytical techniques employed for characterization included gas chromatography/mass spectrometry (GC/MS), liquid chromatography/electrospray ionization coupled with Orbitrap high-resolution MS (LC/ESI-HRMS), multistage MS (ESI-MS^n), and nuclear magnetic resonance (NMR).

EXPERIMENTAL

Chemicals and reagents

Water, acetonitrile, formic acid, chloroform, ethyl acetate, methanol, deuterated chloroform ($CDCl_3$) and tetramethylsilane (TMS) were purchased from Sigma-Aldrich (Milan, Italy); ammonium formate was obtained from Agilent Technologies (Santa Clara, CA, USA).

Sample preparation

For GC/MS analysis

Sample preparation was carried out by dissolving about 2.5 mg of the seized powder in 1 mL of ethyl acetate, and the solution obtained was diluted ten-fold prior to GC/MS analysis.

For LC/ESI-HRMS and ESI-MS^n analysis

A methanolic solution of the seized powder (1 mg in 5 mL) was further ten-fold diluted with water/methanol (80:20) and injected into the LC/ESI-HRMS system, or ten-fold diluted with methanol and infused into the ESI-MS^n system.

For NMR analysis

The seized powder (*ca* 10 mg) was dissolved in $CDCl_3$ (0.5 mL). The filtrate was submitted to ^1H and ^{13}C NMR analyses.

Instrumental parameters

For GC/MS

GC/MS analyses were performed on an Agilent 7890 series II/5975 GC/MS quadrupole mass spectrometer operating in electron ionization (EI, 70 eV) and full-scan (m/z 40–600) acquisition mode (Agilent Technologies, Cernusco sul

Naviglio, Italy). Injection (1 µL, 250 °C) was in split (1:20) or splitless (1 min) mode, with a carrier gas (He) flow rate of 1 mL/min. An Agilent HP-5MS UI (ultra inert, 30 m × 0.25 mm, 0.25 µm film thickness) capillary column was used and the oven temperature was programmed from 50 °C (0.5 min) to 200 °C at 30 °C/min, then to 300 °C (5 min) at 10 °C/min. The interface temperature was 280 °C, and the source temperature was 250 °C. The electron multiplier was set at +300 V with respect to the autotune value.

For LC/ESI-HRMS

The LC/ESI-HRMS instrument comprised a Accela 1250 UHPLC system (Thermo Fisher Scientific, Bremen, Germany) equipped with a Hypersil Gold PFP analytical column (2.1 × 100 mm, 1.9 µm particle size; Thermo Fisher Scientific) and coupled to a single-stage Exactive high-energy collisional dissociation (HCD) Orbitrap mass spectrometer (Thermo Fisher Scientific), with a heated electrospray ionization HESI-II Ion Max source. Samples were injected by means of a HTC PAL autosampler (CTC Analytics AG, Zwingen, Switzerland). Mobile phase A was water with 0.05% formic acid and 10 mM ammonium formate, and mobile phase B was acetonitrile with 0.05% formic acid. The analytical column was maintained at 40 °C and the sample injection volume and temperature were 5 µL and 15 °C, respectively. The flow rate was set to 400 µL/min. The mobile phase gradient was: 99% A for 1 min, linear gradient to 70% B in 6.5 min, linear gradient to 100% B in 0.5 min, held for 2.0 min; column re-equilibration was performed with a linear

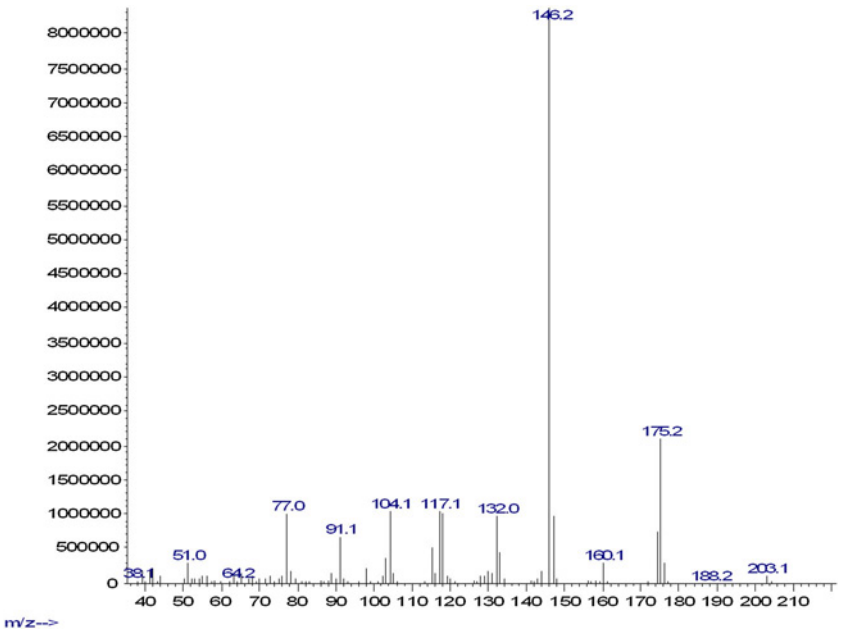

Figure 2. EI full-scan mass spectrum of deschloroketamine.

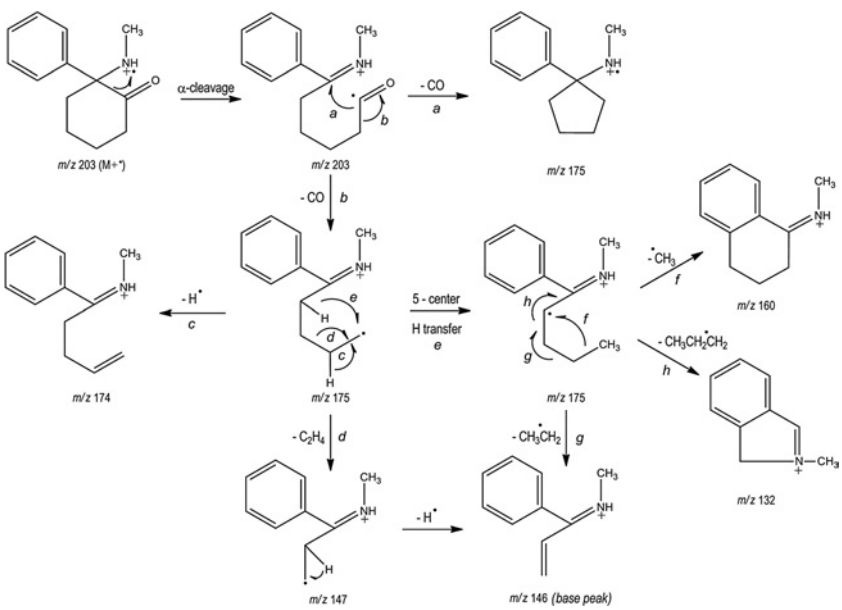

Figure 3. Postulated EI fragmentation pathways of deschloroketamine.

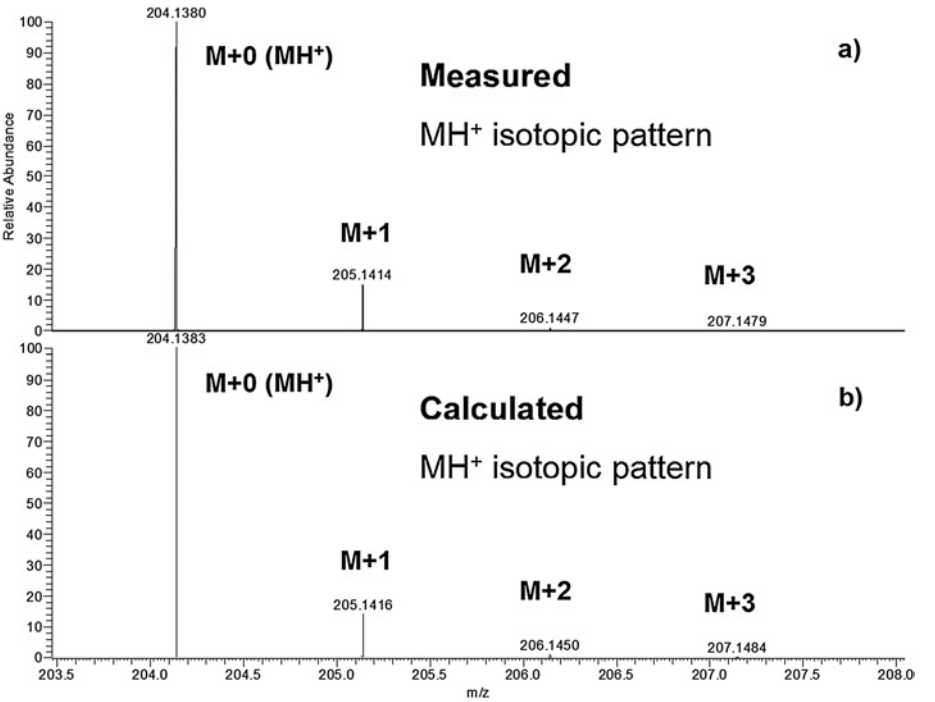

Figure 4. (a) LC/ESI-HRMS experimental isotopic pattern of deschloroketamine MH^+ ions and (b) calculated isotopic pattern of ions with the elemental composition $C_{13}H_{17}NO$.

gradient to 99% A in 3.0 min, held for 3.0 min. The ESI-II Ion Max source, operating in positive ion mode, was heated at 260 °C. The spray voltage was 2500 V, the sheath (N_2) and auxiliary gas (N_2) flow rates were 40 and 5 arbitrary units, respectively, and the ion transfer capillary temperature and voltage were 290 °C and 30 V, respectively. Mass spectrometry analysis was performed by alternating full-scan and 'all-ion fragmentation' (HCD on, collision energy 20 eV) acquisition with a scan range from m/z 100 to 800 at a mass resolution of 100,000. External mass calibration was performed according to the guidelines provided by the instrument supplier every 2 days over the mass range m/z 130–2000.

For ESI-MS^n

ESI-MS^n spectra were obtained using a LCQ Fleet Thermo Fisher Scientific ion trap mass spectrometer equipped with an electrospray ionization (ESI) source, operating in positive ion mode. The diluted methanolic solution of the seized powder was directly infused into the source via a syringe pump at a flow rate of 10 μL/min. The ions were produced using a spray voltage of 3–4 kV and an entrance capillary temperature of 280 °C. Other instrumental parameters were automatically adjusted to optimize the signal-to-noise ratio. Tandem mass spectrometry (MS^n) experiments were performed by resonant excitation of the ion of interest through a supplementary radiofrequency (r.f.) voltage in the range 10–35% of its maximum value (5 V peak-to-peak). The precursor ion isolation width was set at 4 m/z units.

For NMR

^{1}H and ^{13}C NMR spectra were recorded on a AMX-300 instrument (Bruker Italia, Milano, Italy) operating at 300.13 MHz for ^{1}H and 75.43 MHz for ^{13}C, and equipped with a 5 mm reverse probe with z-gradient. All spectra were recorded at 300 K. An exponential function with LB = 0.5 was applied before Fourier transformation, and the phase and baseline were adjusted with TOPSPIN software (Bruker Biospin). A standard *cosygpmfqf* pulse program provided by Bruker was applied for two-dimensional COSY experiments.

RESULTS AND DISCUSSION

GC/MS analysis

The EI full-scan mass spectrum of deschloroketamine is shown in Fig. 2, and the postulated EI fragmentation pathway is shown in Fig. 3. The mass spectrum of deschloroketamine is similar in appearance to those of ketamine and methoxetamine and, because of the similarity of the three structures, the fragmentation pathway of deschloroketamine is expected to be consistent with those proposed for ketamine[13] and methoxetamine.[14] Initial ionization at the amine nitrogen, giving rise to the molecular ion at m/z 203, is followed by alpha cleavage (cleavage of the C^1–C^2 bond in the cyclohexanone moiety), leaving the charge stabilized on the N atom. Neutral loss of CO to produce the ion at m/z 175 can occur with ring closure (path *a* in Fig. 3), or ring opening (path *b*) with the formation of a distonic ion. Loss of a hydrogen radical from these ions (path *c*) results in the ion at m/z 174, while neutral loss of ethylene (path *d*) yields the ion at m/z 147, which in turn can lose a hydrogen radical leading to the highly conjugated, and therefore stable, base peak at m/z 146. On the other hand a five-centered rearrangement of the distonic ion, with H transfer to move the radical site nearer to the N atom (path *e*), may lead to further fragmentation, i.e. the loss of a methyl radical and ring closure (path *f*) to give ions at m/z 160, the loss

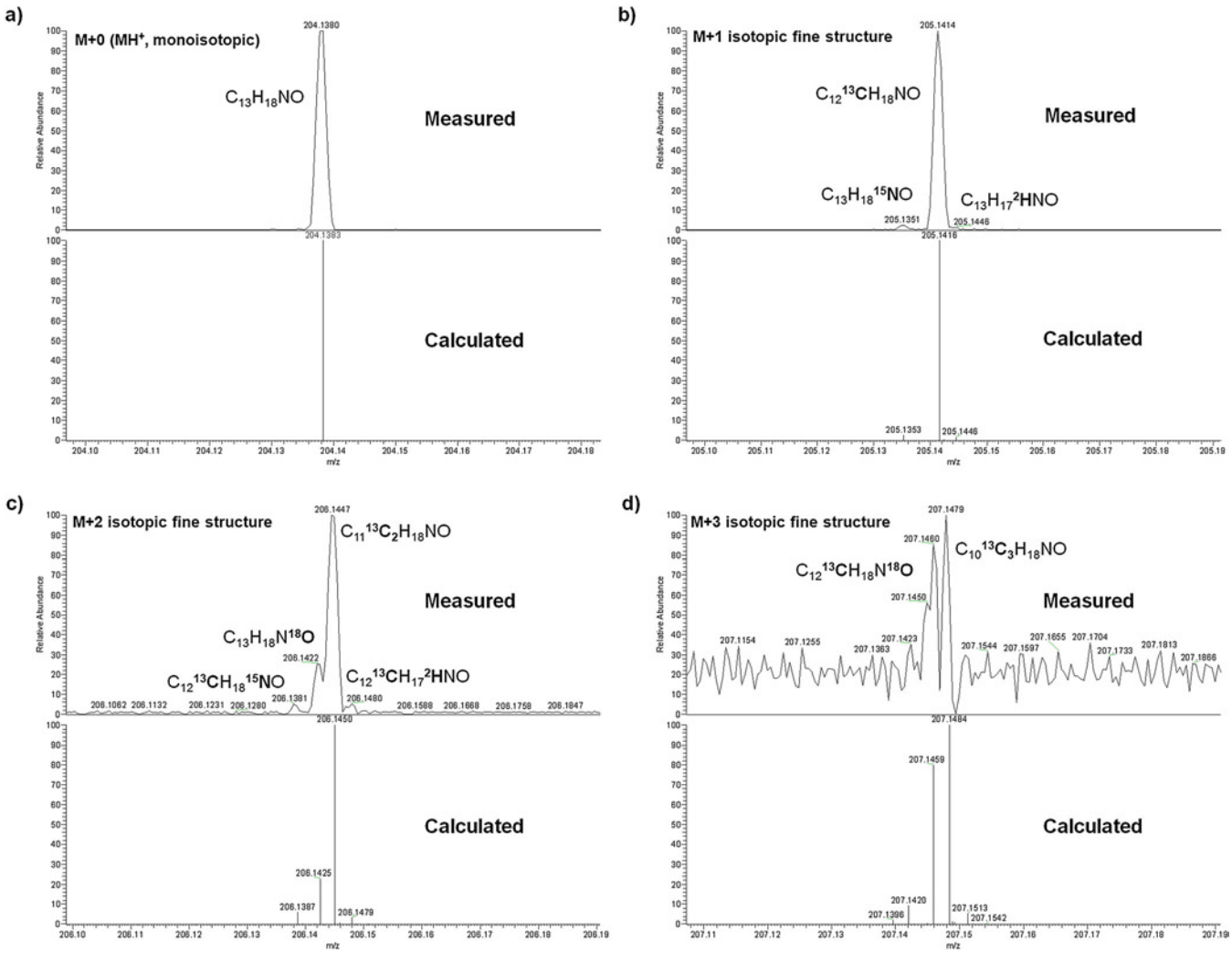

Figure 5. Isotopic fine structures of (a) deschloroketamine MH^+ ions (M + 0), (b) M + 1 isotopic peak, (c) M + 2 isotopic peak, and (d) M + 3 isotopic peak, for both the experimental and the calculated isotopic patterns.

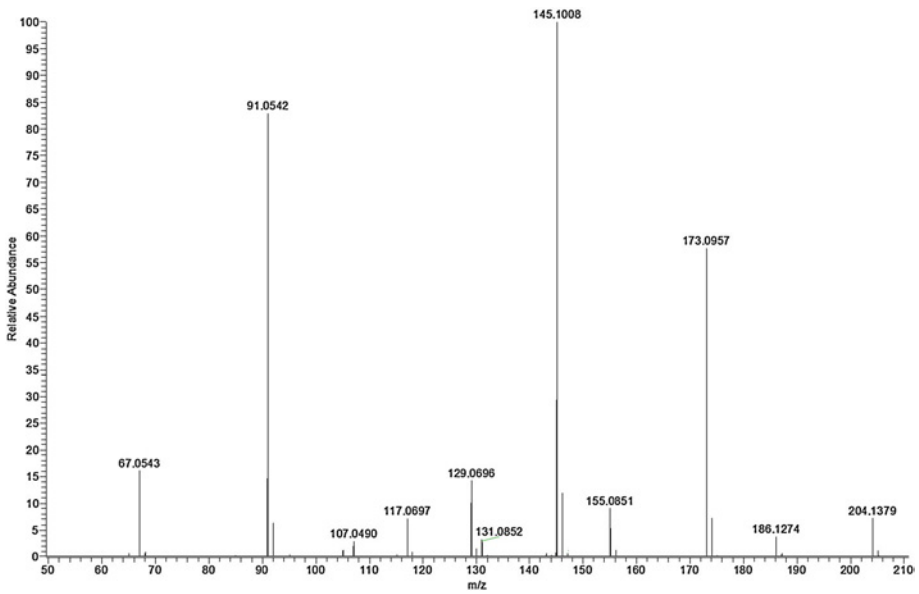

Figure 6. LC/ESI-HRMS mass spectrum, obtained by collision-induced dissociation (HCD on, 20 eV), of deschloroketamine MH^+ ions.

of an ethyl radical (path *g*) to give again the base peak at *m/z* 146, and the loss of a propyl radical and ring closure (path *h*) to give the ion at *m/z* 132. A six-membered ring structure is suggested for the ion at *m/z* 160, as this seems to be less strained than the cyclopropyl ring proposed for the corresponding ion in the EI spectrum of ketamine.[13]

LC/ESI-HRMS and ESI-MS^n analyses

The analytical workflow for deschloroketamine LC/ESI-HRMS measurements, already adopted for the analytical characterization of other NPS,[6,15] consisted of: (i) accurate mass measurements of the ESI-generated MH^+ ion in full scan mode; (ii) comparison of the experimental and calculated MH^+ isotopic patterns[16,17]; and (iii) examination of the isotopic fine structure (IFS) of the M + 1, M + 2, M + 3 isotopic peaks relative to the monoisotopic M + 0 peak.[18,19] The results obtained are summarised as follows.

(i) The measured mass of the MH^+ ion was 204.1380, as opposed to the calculated mass for the MH^+ $C_{13}H_{18}NO$ ion of deschloroketamine of 204.1383, giving a mass accuracy of 1.47 ppm. This measurement is in agreement with the elemental formula of deschloroketamine, $C_{13}H_{17}NO$.

(ii) The experimental and calculated isotopic patterns of deschloroketamine MH^+ ions are shown in Figs. 4(a) and 4(b), respectively. They are fully superimposable, both for their measured/exact mass values and for their relative abundances. The relative isotopic abundance (RIA), i.e. the ratio of the M + 1 (mainly due to ^{13}C isotopes) and the monoisotopic M + 0 ions abundances, was computed for both the experimental and the calculated isotopic patterns. The RIA error, expressed as (experimental RIA – calculated RIA)/calculated RIA × 100, was 3.69%, a value that is considered to be highly diagnostic.[18] These findings strongly support the assignment of the elemental formula $C_{13}H_{17}NO$ to the seized drug.

(iii) Figures 5(a)–5(d) show the IFS of the M + 1, M + 2, M + 3 isotopic peaks relative to the monoisotopic M + 0 peak (deschloroketamine MH^+ ions) for both the experimental and the calculated isotopic patterns. The measured isotopic peaks were fully resolved at the instrumental resolving power of 100,000 and their fine structures, because of the contribution of ^{13}C, ^{2}H, ^{15}N, ^{18}O isotopes, were in accordance with theoretical values. In particular, Fig. 5(b) shows that the experimental M + 1 peak is composed of the $C_{13}H_{18}\mathbf{^{15}N}O$, $C_{12}\mathbf{^{13}C}H_{18}NO$, $C_{13}H_{17}\mathbf{^{2}H}NO$ ions, and that their measured mass values and relative abundances are in full agreement with the theoretical mass values and abundances. Similarly, Fig. 5(c) shows the experimental IFS of the M + 2 peak, due to the $C_{12}\mathbf{^{13}C}H_{18}\mathbf{^{15}N}O$, $C_{13}H_{18}N\mathbf{^{18}O}$, $C_{11}\mathbf{^{13}C_2}H_{18}NO$, and $C_{12}\mathbf{^{13}C}H_{17}\mathbf{^{2}H}NO$ ions, superimposable to the calculated one, both for their measured/exact mass values and for their relative abundances. Lastly, the experimental IFS of the M + 3 peak (main ions $C_{12}\mathbf{^{13}C}H_{18}N\mathbf{^{18}O}$ and $C_{10}\mathbf{^{13}C_3}H_{18}NO$) is depicted, together with the corresponding calculated one, in Fig. 5(d). These findings confirm the elemental formula $C_{13}H_{17}NO$ for deschloroketamine.

The collision-induced product ions of the MH^+ precursor ion were studied by both HRMS and MS^n. Figure 6 shows the LC/ESI-HRMS mass spectrum, obtained by CID (HCD on, 20 eV) of the deschloroketamine MH^+ ion. Figures 7(a), 7(b) and 7(c) show the ESI-MS^n mass spectra obtained by isolation and fragmentation of the deschloroketamine MH^+ ion at *m/z* 204; the product ion at *m/z* 173 arising from the MH^+ ion at *m/z* 204; and the product ion at *m/z* 145 arising from the *m/z* 173 ion, respectively.

The postulated fragmentation pattern of deschloroketamine MH^+ ions, derived from both HRMS and MS^n experiments, is reported in Fig. 8, and parallels the fragmentation pattern reported for ketamine.[20] Overall, while the fragmentation processes observed under EI conditions are mainly due to radical losses, all the collision-induced fragmentations of the ESI-generated MH^+ species involve the losses of neutral moieties resulting in even-electron product ions. Two different fragmentation pathways originate from two different deschloroketamine MH^+ precursor ions, formed by protonation on the two basic sites present in the molecule (the N and O atoms). On the one hand, loss of water gives the ion at *m/z* 186.1274 ($C_{13}H_{16}N$) while, on the other, loss of CH_3NH_2 gives rise to the ion at *m/z* 173.0957 ($C_{12}H_{13}O$), with further loss of water yielding the ion at *m/z* 155.0851 ($C_{12}H_{11}$). Loss of CO from *m/z* 173.0957 leads to the formation of the ion at *m/z* 145.1008 ($C_{11}H_{13}$). The ions at *m/z* 117.0697 (C_9H_9), 91.0542 (C_7H_7), and 67.0543 (C_5H_7) are obtained from the fragmentation/rearrangement of *m/z* 145.1008, through losses of C_2H_4, C_4H_6, and C_5H_7, respectively. The mass accuracy was better than 2 ppm for all ions.

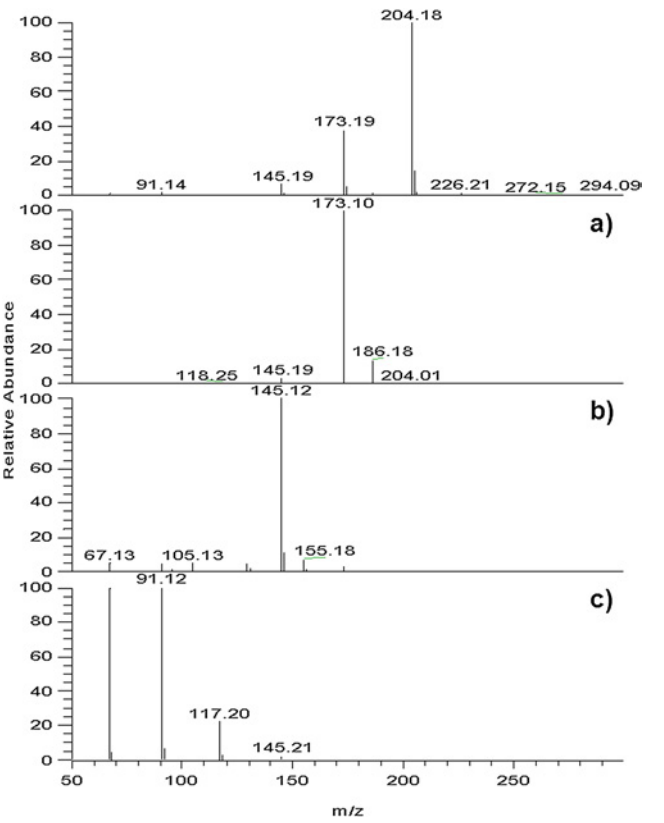

Figure 7. ESI-MS^n mass spectra, obtained by isolation and fragmentation of (a) the deschloroketamine MH^+ ion at *m/z* 204, (b) the ion at *m/z* 173 arising from *m/z* 204, and (c) the ion at *m/z* 145 arising from *m/z* 173.

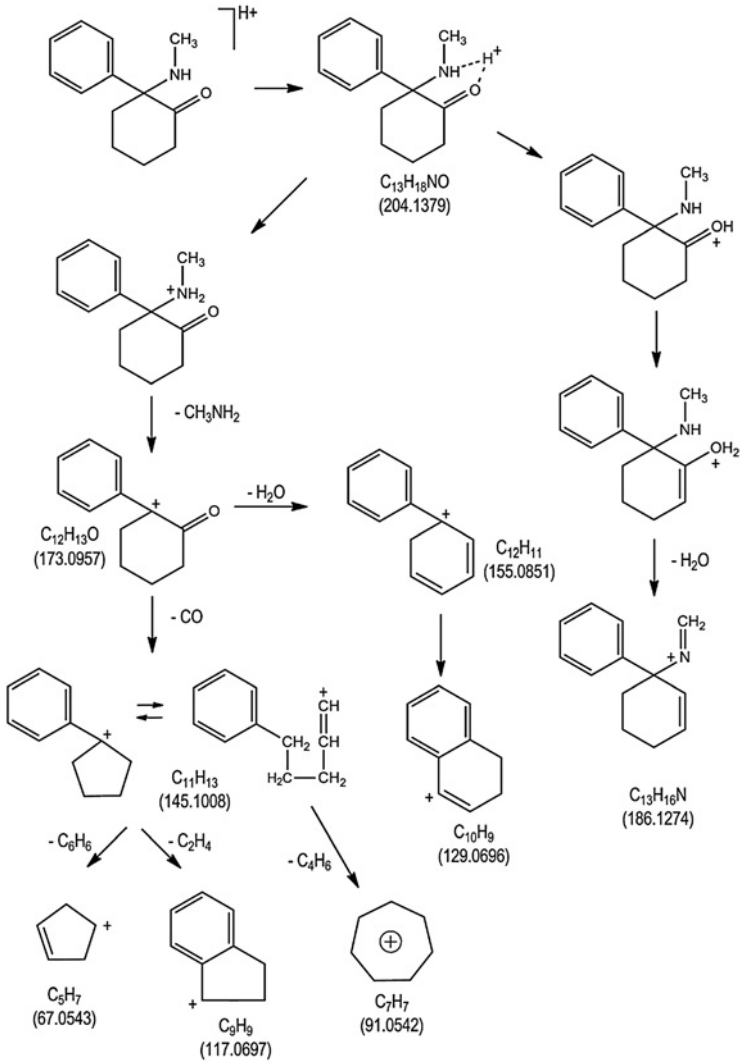

Figure 8. Postulated fragmentation pattern of deschloroketamine MH^+ ions, inferred from both HRMS and MS^n fragmentation experiments.

NMR analysis

Mono-dimensional (^1H and ^{13}C) and two-dimensional (^1H-^1H COSY) NMR measurements were carried out to confirm the chemical structure of the analyte following MS measurements. The assignments of the ^1H and ^{13}C chemical shifts, expressed in ppm relative to TMS, are reported in Table 1 and representative spectra are shown in Figs. 9–11. The ^1H NMR spectrum of the seized powder (Fig. 9) shows that deschloroketamine is supplied as its chlorohydrate salt. The two unequivalent amine protons show broad singlets at 10.22 and 9.91 ppm (marked with 1 in the illustration) that are both coupled with the methylamine protons (marked with 1′), as indicated from the ^1H-^1H COSY map (Fig. 10, full lines). In addition, a set of aromatic proton signals (H_{ar}) at *ca* 7.50 ppm (integration for five protons) and a set of aliphatic proton signals (3–6) in the range 3.19–1.67 ppm (integration for eight protons) confirm the presence of a phenyl group

Table 1. ^1H and ^{13}C NMR data of deschloroketamine

^1H signal	ppm (integration)	^{13}C signal	ppm
H1	10.22 (bs) (1H) 9.91 (bs) (1H)		
H1′	2.47 (t; $^3J_{HH}$ = 5.45 Hz) (3H)	C1′ C3–C6	27.46 39.30, 32.86, 27.11, 21.72
		C2 (C = O)	204.62
H3 – H6	3.19 – 1.67 (8H)		
		C7	71.98
H_{ar}	7.54 – 7.43 (5H)	C_{ar}	130.18, 129.84, 128.62

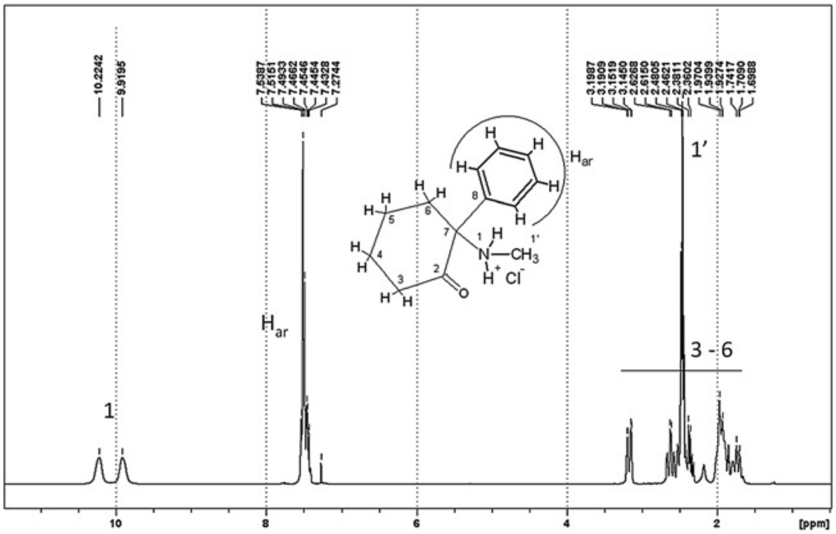

Figure 9. ^{1}H NMR of deschloroketamine in $CDCl_3$.

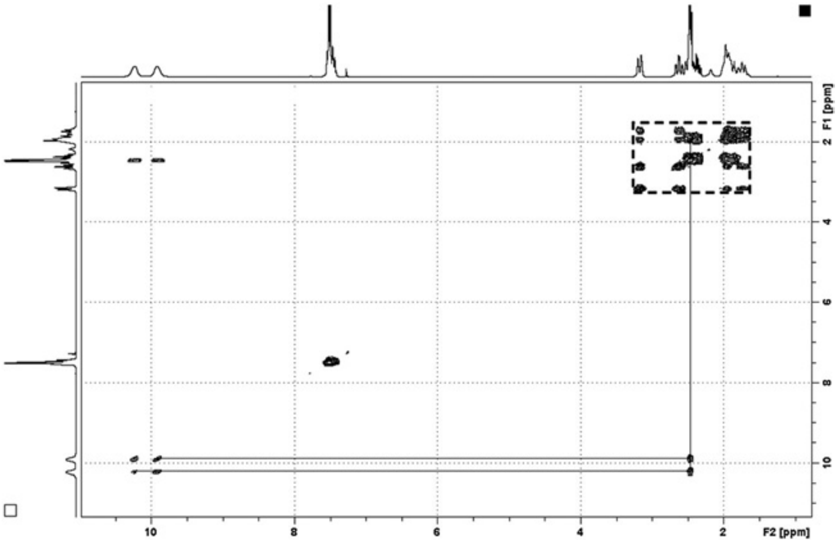

Figure 10. ^{1}H-^{1}H COSY NMR map of deschloroketamine in $CDCl_3$.

and of a keto-amine ring. The ^{1}H-^{1}H COSY map (Fig. 10, dotted frame) shows that the aliphatic protons are all coupled. The ^{13}C NMR spectrum of the seized drug (Fig. 11) shows the distinctive keto-amine carbon at 204.62 ppm (marked with 2), the quaternary carbon (marked with 7) at 71.98 ppm and five signals due to aliphatic carbons in the range 39.31–21.72 ppm. The triplet signal around 77 ppm is due to the $CDCl_3$ solvent.

For comparison purposes, the ^{1}H and ^{1}H-^{1}H COSY map of the chloro-hydrate salt of ketamine was collected under similar experimental conditions. The ^{1}H NMR profile (spectrum not shown) is consistent with that of deschloroketamine. It shows: (i) two unequivalent amine protons at 9.58 and 10.53 ppm coupled with the methylene protons; (ii) a set of aromatic signals in the 8.04–7.44 ppm region (the enlarged window compared with that shown by deschloroketamine is due to the presence of the chloro substituent in the aromatic ring); and (iii) a set of aliphatic signals in the 3.55–1.56 ppm region. All the aliphatic signals are coupled each other, as evidenced in the ^{1}H-^{1}H COSY contour map (map not shown).

2-Methylamino-2-phenylcyclohexanone, the compound that we named deschloroketamine, is not, to the best of our knowledge, an explicitly controlled substance in Italy, or probably in most European countries. From this case, as well as information from the Spanish Energy Control NGO alert,[11] we know that deschloroketamine is sold, knowingly or not, as ketamine in the recreational drug market. However, apart from the generic information that this compound could be more potent and longer lasting than ketamine,[10,12] no extensive data on its psychoactive effects and related toxicity are available at the moment from the scientific community. For these reasons, consumption of this substance should be avoided, at least until more information is available about its health effects.[11]

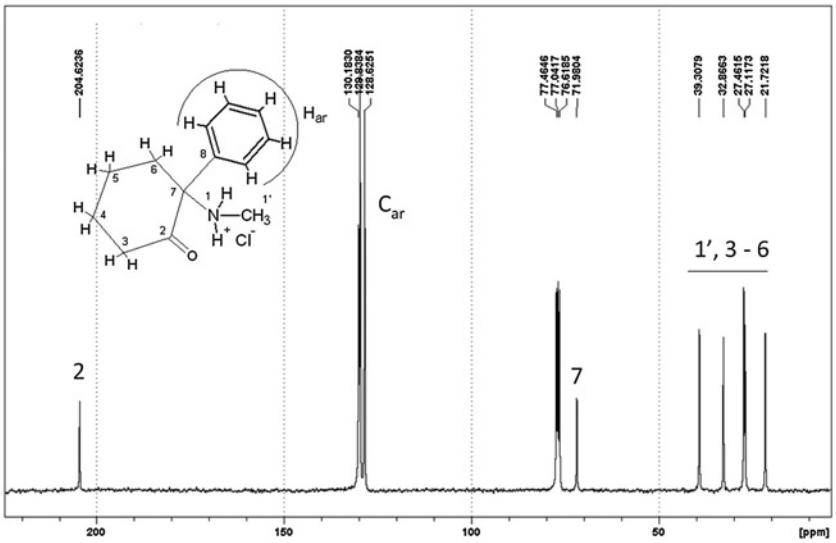

Figure 11. ^{13}C NMR of deschloro-ketamine in $CDCl_3$.

CONCLUSIONS

This study has shown that the identification of NPS, at least in seized materials, can be achieved by the combination of multiple uncorrelated analytical techniques, in spite of the lack of reference standards or analytical data from the scientific literature. In this study the molecular structure of a new designer drug and ketamine analog, named deschloroketamine, was first investigated through the study of characteristic fragment ions obtained from GC/MS analysis. Then, HRMS analysis allowed accurate mass measurement of the deschloroketamine MH^+ ion to be obtained, with a mass accuracy of 1.47 ppm; fully superimposable experimental and calculated MH^+ isotopic patterns, with a RIA value of 3.69%; and the IFS of the M + 1, M + 2, M + 3 isotopic peaks relative to the monoisotopic M + 0 peak completely in accordance with theoretical values. These findings enabled us to obtain the elemental compositional formula of the seized drug. Furthermore, the examination of the collision-induced product ions of the MH^+ precursor ion obtained under both HRMS and MS^n conditions, as well as the study of both mono-dimensional and two-dimensional NMR, enabled the full characterization of the molecular structure of deschloroketamine.

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