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25C-NBOMe – New potent hallucinogenic substance identified on the drug market[☆]

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ABSTRACT

This publication reports analytical properties of a new hallucinogenic substance identified in blotter papers seized from the drug market, namely 25C-NBOMe [2-(4-chloro-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine]. The identification was based on results of comprehensive study including several analytical methods, *i.e.*, GC–EI–MS (without derivatization and after derivatization with TFAA), LC–ESI–QTOF–MS, FTIR and NMR. The GC–MS spectrum of 25C-NBOMe was similar to those obtained for other representatives of the 25-NBOMe series, with dominant ions observed at $m/z = 150, 121$ and 91. Fragment ions analogic to those in 2C-C (4-chloro-2,5-dimethoxy- β -phenylethanamine) were also observed, but their intensities were low. Derivatization allowed the determination of molecular mass of the investigated substance. The exact molecular mass and chemical formula were confirmed by LC–QTOF–MS experiments and fragmentation pattern under electrospray ionization was determined. The MS/MS experiments confirmed that the investigated substance was N-(2-methoxy)benzyl derivative of 2C-C. The substance was also characterized by FTIR spectroscopy to corroborate its identity. Final elucidation of the structure was performed by NMR spectroscopy.

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1. Introduction

25C-NBOMe is a short name for 2-(4-chloro-2,5-dimethoxyphenyl)-N-[(2-methoxyphenyl)methyl]ethanamine. Alternative abbreviations used for this substance include 2C-C-NBOMe and NBOMe-2C-C, while its street names are *C-Boom*, *Cimbi-82*, *Pandora* and *Dime* [1]. The synthesis of 25C-NBOMe was first reported in scientific literature in 2011 by Ettrup et al. [2,3]. It was derived from the psychedelic phenethylamine 2C-C (4-chloro-2,5-dimethoxyphenethylamine) by substitution on the amine nitrogen with a 2-methoxybenzyl (BOMe) group. This synthesis can be realized in two ways: by reductive amination of 2-methoxybenzaldehyde with 2C-C using sodium borohydride [4] or reductive amination of 2-hydroxybenzaldehyde with the same parent phenethylamine and further methylation of the hydroxy group [2]. Fig. 1 displays the structural relationship between 2C-C and 25C-NBOMe.

25C-NBOMe is a representative of a new class of hallucinogens, called 25-NBOMe or simply NBOMe. This name is used for various

analogs of 2C-series phenethylamine designer drugs. The NBOMe compounds have nearly no history of human use prior to 2010 when they first became available online [5]. Blotter papers and powders containing psychedelics started to enter the Polish drug scene in 2011 and a number of new tryptamine and phenethylamine derivatives were detected in the Institute of Forensic Research (IFR) in Krakow. Of phenethylamines, 2C-N (2,5-dimethoxy-4-nitrophenethylamine) [6], 2C-G (2,5-dimethoxy-3,4-dimethylphenethylamine) [7] and three representatives of the 25-NBOMe series containing alkyl group at position 4 of the benzyl ring [8] were first identified. Blotter papers containing 25C-NBOMe also appeared on the market in 2011. Recently, there have been several online shops offering this substance. In the first half of 2012, seven different sorts of blotters impregnated with 25C-NBOMe were seized by the police and delivered for the analysis in the IFR. Exemplary blotter papers with 25C-NBOMe are presented in Fig. 2. In some blotters, 25C-NBOMe was mixed with 25D-NBOMe (2-(2,5-dimethoxy-4-methyl phenyl)-N-[(2-methoxyphenyl)methyl]ethanamine) and/or DOI (2,5-dimethoxy-4-iodoamphetamine). 25C-NBOMe was also discovered to be on sale as ‘legal LSD’ in New Zealand in early 2012 [9,10]. According to the information found in the Internet [1], 25C-NBOMe has also been available as powder tabs or liquid in ‘LSD style’ dropped bottles.

The action of 25C-NBOMe results from the fact that it is a potent partial agonist for the serotonin 2A (5-HT_{2A}) receptors. These receptors are implicated in the pathophysiology of depression and

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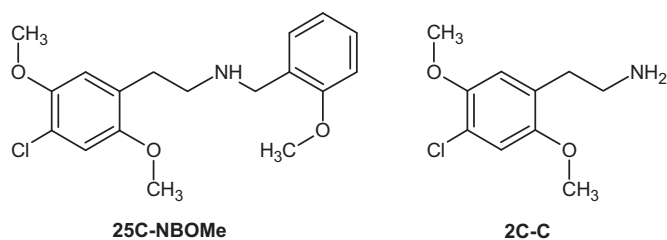


Fig. 1. Chemical structures of 25C-NBOMe and 2C-C.

schizophrenia. Their stimulation is responsible for the hallucinogenic effects of many recreational drugs including lysergic acid diethylamide (LSD) and representatives of 2C-series [11–13]. 25C-NBOMe showed nanomolar affinity toward the 5-HT_{2A} receptor; its *in vitro* 5-HT_{2A} receptor agonistic binding affinity was 2.89 ± 1.05 nM [2].

The aforementioned results of the scientific study performed *in vitro* indicating potential of 25C-NBOMe as a hallucinogen have been confirmed by users reports on ‘self-experiments’ published on Internet fora [14–18]. However, those reports are subjective and should be treated with great precaution because the users could have taken some other drug for 25C-NBOMe. Reported hallucinogenic effects after 25C-NBOMe cover extreme patterning, vibrant coloring, strong sound distortion (sounds leaking in and out of rooms and into the user), very strong electric spasmodic body high. Some users have been reported to have less ‘after effects’ and generally less unwanted side effects than traditional compounds from the 2C-series. Described side effects included panic attacks, loss of location and time, and slight nausea.

25C-NBOMe is a hallucinogen and, as common with this class of substances, recommended routes of administration are strictly parenteral. Reports from human users suggest 25C-NBOMe to be an active hallucinogen at a dose of as little as 200–1000 µg when administered intranasally or sublingually; and from 50 to 500 µg when smoked (as freebase), making it only slightly less potent than LSD. It reportedly displays relatively weak activity when dosed orally. The effects of insufflation of 25C-NBOMe are light after 50–200 µg, mild after 200–350 µg, strong after 350–700 µg and very strong after higher doses. When administered sublingually, the threshold effect is achieved after 100–250 µg, mild – 250–450 µg, strong – 450–800 µg, very strong – over 800 µg. ‘Come up’ appears in 1 h, and plateau lasts 3–4 h. Total duration of action is up to 4–10 h [19].

25C-NBOMe is not controlled by the United Nations drug conventions [20,21], therefore it is legally available in countries in which drug law is based directly on these treaties. On the other hand, some countries modified their drug law or have applied other acts to control novel psychoactive substances. For example, in Poland 25C-NBOMe is treated as ‘drug substitute’ and its manufacture, marketing and even advertising is banned. It was also withdrawn from official sale in New Zealand because it was recognized to be substantially similar in chemical structure to the illegal hallucinogen DOB (4-bromo-2,5-dimethoxyamphetamine) [22]. In contrast, 25C-NBOMe is uncontrolled in the United Kingdom, as *N*-benzyl derivatives of phenethylamine are not

covered by the phenethylamine derivatives clause of the Misuse of Drugs Act 1971 [23]. It is also uncontrolled in the USA at federal and state level, though, according to some experts, it may contravene the Federal Analog Act due to its structural and functional similarity to controlled substance 2C-B (4-bromo-2,5-dimethoxyphenethylamine).

This paper reports analytical properties of 25C-NBOMe. Its structure elucidation was carried out by means of gas chromatography coupled to mass spectrometry (GC–MS) without derivatization and after derivatization with trifluoroacetic anhydride (TFAA), liquid chromatography coupled to quadrupole-time-of-flight mass spectrometry (LC–QTOF–MS), Fourier transformed infrared spectroscopy (FTIR) and by nuclear magnetic resonance (NMR).

2. Materials and methods

2.1. Material and reagents

The investigated materials were absorbent blotter papers with printed artwork (as shown in Fig. 2).

Methanol and acetonitrile (HPLC grade, purity (GC) $\geq 99.9\%$), formic acid (analytical grade, 89–91%) and TFAA were supplied by Merck (Darmstadt, Germany). Analytical grade ethyl acetate (purity $\geq 99.5\%$) and chloroform (purity $\geq 99.0\%$) were purchased from POCH (Gliwice, Poland) and Lach-Ner (Neratovice, Czech Republic), respectively. Deionized water was obtained by reverse diffusion in a Millipore system.

2.2. Sample preparation

For GC–MS and LC–MS:

A blotter paper was soaked in 0.5 ml methanol for 6 h. For GC–MS analysis, the filtered supernatant was introduced via an auto injector using an injection volume of 3 µl. For LC–MS analysis, the supernatant was diluted with 0.1% (v/v) formic acid in water and introduced via the auto injector using an injection volume of 5 µl.

For GC–MS with derivatization, FTIR and NMR:

Fifteen blotter papers were soaked in 1 ml methanol in an ultrasonic bath for 1 h. The obtained extract was evaporated to dryness under a stream of air.

Derivatives were prepared by dissolving dry extracts separately in 100 µl of derivatizing agent (trifluoroacetic anhydride (TFAA):chloroform, 1:1, v:v), and, after vortex mixing, the reaction mixture was incubated in a capped tube at 70 °C for 40 min. After cooling to room temperature, the samples were evaporated to dryness under a stream of air at 37 °C and reconstituted with 80 µl of ethyl acetate.

For FTIR analysis, the dry extract was placed on the microscope stage of the spectrometer, in the infrared beam, and the spectrum was measured by the transmission technique.

For NMR analysis, the dry extract was dissolved in deuterated chloroform (CDCl₃).

2.3. Instrumentation

GC–MS analysis was performed using an HP 6890 series gas chromatography system coupled to a 5973N series mass selective detector manufactured by Agilent (Santa Clara, CA, USA). The extracts were injected automatically in splitless mode. Chromatographic separation was carried out on an HP-5MS capillary column (30 m × 0.25 mm × 0.25 µm) and helium at a constant flow rate of 1 ml/min was used as the carrier gas. The initial column temperature (75 °C) was maintained for 1 min, then increased linearly at a rate of 25 °C/min to 280 °C, and finally maintained for 20.8 min. The GC injector and the transfer line were maintained at 280 °C. The spectrometer was operated in electron impact mode (EI). The temperatures of the ion source and quadrupole were 230 °C and 150 °C, respectively. Ionization energy was set at 70 eV and positive ions were analyzed. Acquisition was carried out in scan mode from 29 to 600 amu. Under these conditions, the retention time for 25C-NBOMe was 11.7 min, whereas its TFAA derivative was eluted at 11.9 min.

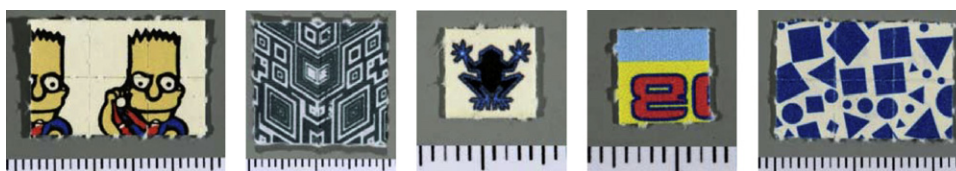


Fig. 2. The blotter papers containing 25C-NBOMe.

LC-QTOF-MS analysis was carried out using a liquid chromatograph 1200 Series Instrument coupled with a 6520 Accurate-Mass Q-TOF LC/MS detector (Agilent Technologies, Santa Clara, CA, USA). Chromatographic separation was performed at 35 °C with an Ascentis Express C18 (7.5 cm × 2.1 mm × 2.7 μm) column (Supelco). For gradient elution the mobile phases 0.1% formic acid in water (A) and 0.1% formic acid in acetonitrile (B) were used with the time program: 0 min – 5% B, linear to 33% B at 11 min, linear to 37% B at 15 min, back to 5% B at 15.2 min and equilibration to 21 min. The flow rate was 0.3 ml/min. The QTOF-MS instrument was operated with an electrospray ion (ESI) source in positive ionization mode. Nitrogen was used as the drying gas at a temperature of 300 °C and flow 10 l/min, and as the nebulizing gas with a pressure of 45 psi. Capillary voltage was set at –3000 V and skimmer voltage at 65 V. The fragmentor voltage was set at 100 V or 240 V. The quadrupole was used as an ion guide in MS mode, and for selection of precursor ions with $\Delta m/z = 1.3$ in MS/MS mode. Nitrogen was used as the collision gas in MS/MS mode and collision energy was set at 15 eV. Mass spectra were collected in the range of 50–1000 m/z in both MS and MS/MS modes. Spectra were internally mass-corrected in real time using an automatically introduced reference mass solution containing two compounds: purine ($[M+H]^+ = 121.050873$) and HP-921 – hexakis(1H,1H,3H-tetrafluoropropoxy)phosphazine ($[M+H]^+ = 922.009798$). Under these conditions, the investigated compound was eluted at 12.9 min.

Infrared measurements (FTIR) were performed by means of an FTS 40Pro Fourier-transform infrared (FTIR) spectrometer (BioRad/Digilab, MA), which was equipped with a water-cooled high temperature ceramic source (MIR). It was coupled with a UMA 500 microscope with a 15× objective and an MCT detector. The IR spectrum was obtained by averaging 256 interferograms at 4 cm^{-1} resolution and it was measured by the transmission technique in the range of 600–4000 cm^{-1} .

^1H and ^{13}C NMR spectra of 25C-NBOMe solution in CDCl_3 were recorded on a Bruker Avance III 600 spectrometer, at 600.2 MHz (^1H NMR) or 150.92 MHz (^{13}C NMR). Chemical shifts are given in parts per million (ppm) relative to the solvent signal. Coupling constants (J) are expressed in Hertz (Hz). The following abbreviations are used to designate NMR absorption patterns: bs – broad singlet; s – singlet; d – doublet; m – multiplet.

3. Results and discussion

3.1. GC-MS analysis without derivatization

GC-EI-MS mass spectrum of 25C-NBOMe is presented in Fig. 3a. It was compared to the spectrum of 2C-C (Fig. 3b). As 25C-NBOMe has chlorine atom at position 4 of the benzyl ring,

the characteristic isotope distribution was observed for fragments containing this substituent.

As for other representatives of 25-NBOMe series, the dominant ions in GC-MS spectrum of 25C-NBOMe were observed at $m/z = 121$ (**7**), 150 (**6**) and 91 (**8**) [8]. The spectrum did not contain a signal of the molecular ion, **M**, but there was an ion recorded at $m/z = 304$ (**1**), which corresponded to **M-31**. Such ion can be formed by the loss of methoxy radical from the molecule. In 25C-NBOMe, there are three positions in which the decay may occur. The dissociation of the methoxy radical from 2-methoxybenzyl ring is the most reasonable, because **M-31** ion was not observed in the parent substance, namely 2C-C.

The predominant ion **7** can be formed by the cleavage of the N–C bond yielding 2-methoxybenzyl cation. The ion **6** could be an iminium cation formed by the dissociation of bond between α - and β -carbon atoms. The decay of the same bond may also lead to dissociation of *N*-(methoxybenzyl)methylimine molecule and formation of carbocation observed at $m/z = 186$ (**3**), similar to the parent substance 2C-C.

The cleavage of the C–N bond in the side chain leads to formation of the ion observed at $m/z = 199$ (**2**); however this ion was not intensive. The loss of methoxy radical from ions observed at $m/z = 199$ (**2**) and 186 (**3**) leads to formation of the cations recorded at $m/z = 169$ (**4**) and at $m/z = 155$ (**5**), respectively.

In turn, the ions with $m/z = 91$, 77 and 65 are characteristic for a benzyl ring containing a methyl substituent. Ion **8** ($m/z = 91$) was a tropylium cation, and it was probably formed by the loss of methoxy radical from the predominant ion **7**.

The above-discussed fragmentation processes of investigated compound are shown in Scheme 1.

3.2. GC-MS analysis of TFAA derivative

The derivatization of 25C-NBOMe and 2C-C was carried out using TFAA reagent. GC-EI-MS spectra of these derivatives are shown in Fig. 4.

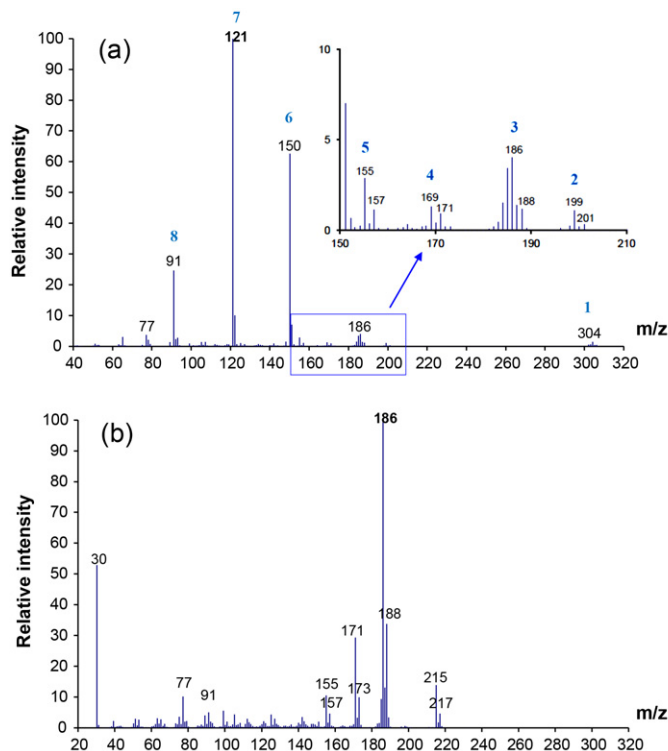
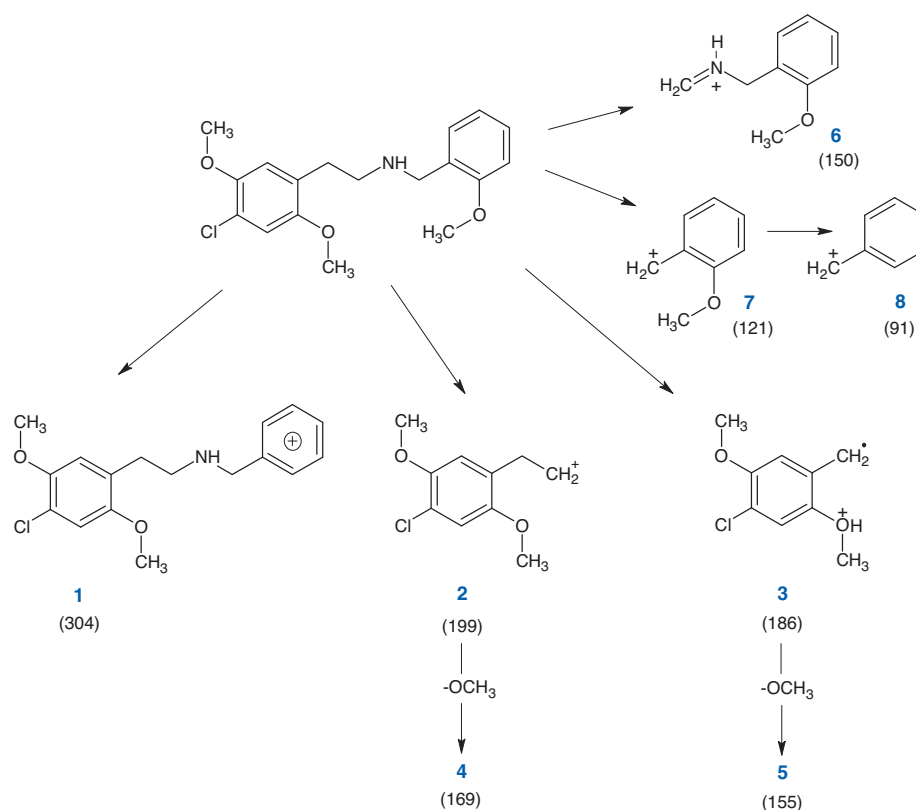


Fig. 3. GC-MS spectra of (a) 25C-NBOMe and (b) 2C-C.



Scheme 1. Proposed fragmentation routes of 25C-NBOMe under EI.

The intensive ion in 25C-NBOMe spectrum was observed at $m/z = 431$, which corresponded to the mono-substituted molecular ion (one hydrogen atom was substituted by the TFAA group).

The dominant ion in the spectrum of the investigated substance was recorded at $m/z = 198$. The radical cation of this mass/charge

ratio can be formed by the cleavage of C–N bond and the loss of $\text{NCOCF}_3\text{C}_8\text{H}_9\text{O}$ moiety. Another dominant ion can be created by dissociation of the bond between α - and β -carbon atoms (the loss of $\text{NCOCF}_3\text{C}_9\text{H}_{11}\text{O}$ moiety). The cation formed in the discussed process was recorded at $m/z = 185$. Further fragmentation of this ion undergoes analogously the process observed for the parent substance 2C-C (the ions were observed at $m/z = 171$ and 155).

3.3. LC-MS

In the first step, the MS analysis was performed at low fragmentor voltage ($U = 100$ V) and exact molecular mass of 25C-NBOMe was confirmed. The protonated molecular ion ($\text{M}+\text{H}^+$) with high accuracy (mass error, $\Delta m = -0.3$ ppm) was observed at $m/z = 336.1360$ (**0**).

The use of higher fragmentor voltage ($U = 240$ V) caused cleavage of some bonds in the molecule, and the main fragments of 25C-NBOMe (**1–4**) were observed. Based on the obtained exact molecular masses, chemical formulas were determined and mass accuracies were calculated (data shown in Table 1). The ion recorded at $m/z = 214.0632$ (**1**) was formed by cleavage of C–N bond, whereas the ion with $m/z = 199.0518$ (**2**) – by cleavage of C–C bond between α - and β -carbon atoms. Those fragments are characteristic for the parent substance 2C-C. The remaining ions **3** and **4** corresponded to *N*-(2-methoxy)benzyl group, which is attached to the nitrogen atom [8].

In the next step, ion **2** was selected for further fragmentation in the MS/MS mode with higher fragmentor voltage ($U = 240$ V) and collision energy $\text{CE} = 15$ eV. These parameters were selected based on an optimization study (data not shown). The spectra of 25C-NBOMe obtained in MS mode ($U = 240$ V, $\text{CE} = 0$ eV) and MS/MS mode ($U = 240$ V, $\text{CE} = 15$ eV) are presented in Fig. 5a and b. Comparing the fragmentation spectrum of 25C-NBOMe with MS/MS spectrum of 2C-C (Fig. 5c), it was noticed that only

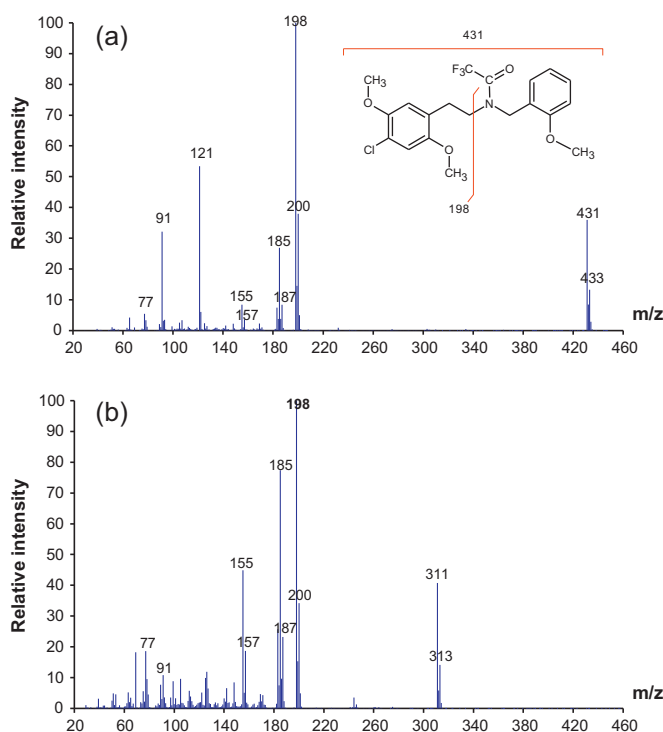


Fig. 4. GC-EI-MS spectra of TFAA derivatives of (a) 25C-NBOMe and (b) 2C-C.

Table 1

The ions observed under ESI-QTOF-MS.

Parameters	Fragment	Formula	Experimental mass	Theoretical mass	Δm [ppm]
I	0	$C_{18}H_{23}ClNO_3^+$	336.1360	336.1361	-0.3
II	1	$C_{10}H_{13}ClNO_2^+$	214.0632	214.0629	1.4
	2	$C_{10}H_{12}ClO_2^+$	199.0518	199.0520	-1.0
	3	$C_8H_9O^+$	121.0649	121.0648	0.8
	4	$C_7H_7^+$	91.0543	91.0542	1.1
III	5	$C_9H_9ClO_2^+$	184.0284	184.0286	-1.1
	6	$C_8H_6ClO_2^+$	169.0047	169.0051	-2.4
	7	$C_{10}H_{12}O_2^+$	164.0837	164.0832	3.0
	8	$C_8H_7ClO^+$	154.0156	154.0180	-15.6

I: $U=100V$, $CE=0eV$; II: $U=240V$, $CE=0eV$; III: $U=240V$, $CE=15eV$.

certain ions (5–8) characteristic for 2C-C were recorded for the investigated sample. It is probably associated with a lower intensity of these ions in 25C-NBOMe, which is out of limit of detection of the applied assay.

Based on the performed experiments, we proposed the fragmentation route for 25C-NBOMe, which is presented in Scheme 2. The fragments correspond to the numbers of ions listed in Table 1. Generally, the fragmentation of ion 2 followed by dissociation of chlorine atom and also by cleavage of methyl and/or methoxy groups. Because the 25C-NBOMe molecule contains more than one methyl and methoxy group, it was not possible to determine exact structures of the product ions (5, 6, 8).

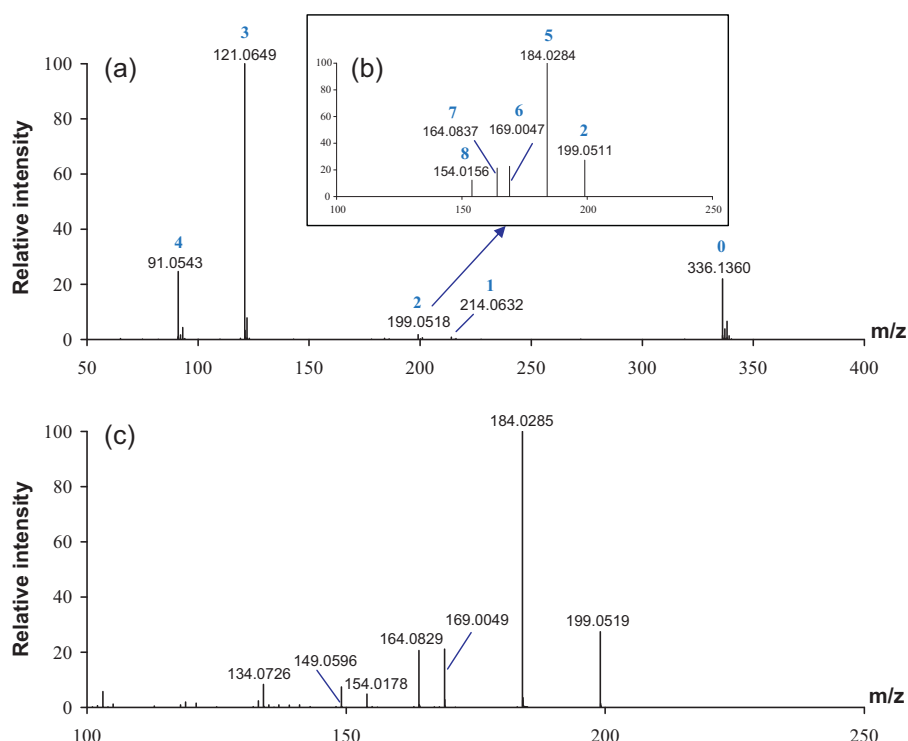
Moreover, the characteristic isotope distribution of the molecules containing chlorine atom was observed and it was compared with the predicted relative isotopic abundance for the pseudomolecular ion $C_{18}H_{23}ClNO_3^+$ in Fig. 6.

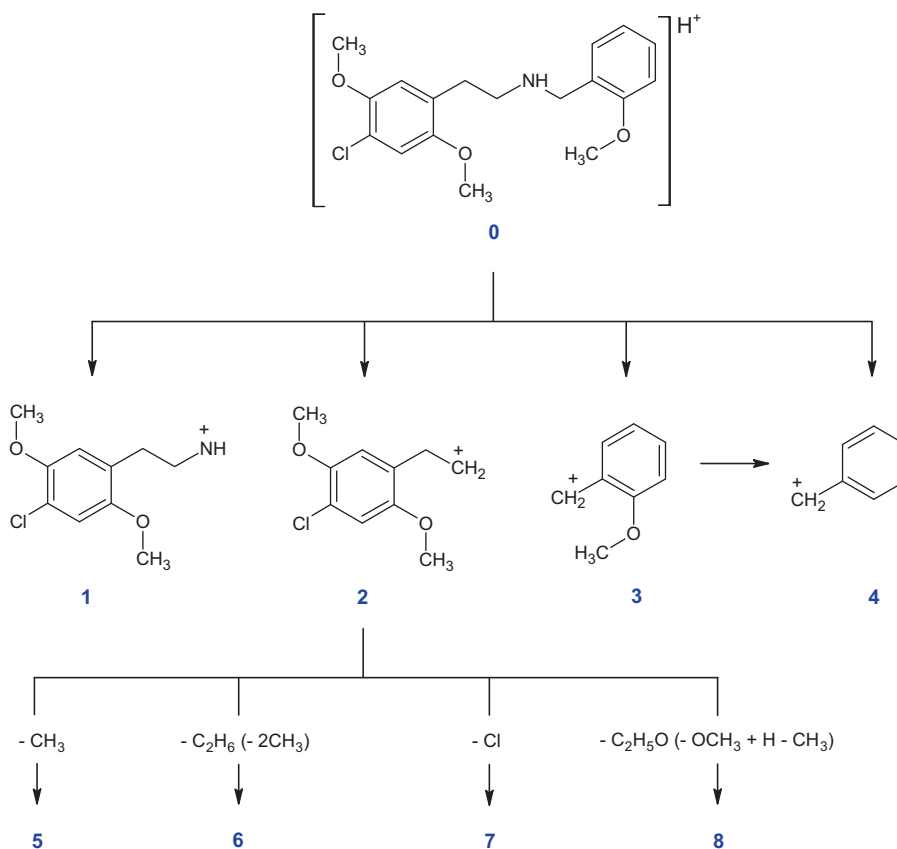
3.4. FTIR

The FTIR spectrum of the examined sample recorded in the 600–4000 cm^{-1} range is presented in Fig. 7.

The presence of one or more aromatic rings in a structure can be readily determined by the C=C and C-H ring-related vibrations. The most important set of bands originating from the aromatic ring C=C stretching vibrations is centered around 1450–1510 cm^{-1} and 1580–1615 cm^{-1} . They usually appear as a pair of band structures, often with some splitting [24,25]. In the analyzed spectrum, two characteristic pairs were observed at 1450–1464 cm^{-1} and 1591–1606 cm^{-1} , respectively. The additional bands recorded around 760–860 cm^{-1} may originate from the C-H out-of-plane bending vibrations of substituted aromatic rings. The structure of these bands is defined by the number and positions of the C-H bonds around the ring, which in turn are related to the nature and number of other substituents on the moiety. The C-H stretch vibrations for methylene groups occurring in saturated aliphatic chain are observed as a multiplicity of strong-to-weak bands, with the dominant band at 2918 cm^{-1} .

In turn, strong peaks observed at 1036 cm^{-1} , 1215 cm^{-1} and 1252 cm^{-1} can be assigned to C–O–C vibrations. Aryl alkyl ethers, as in the case of representatives of 25-NBOMe series, are characterized by the asymmetric C–O–C stretch vibrations near 1250 cm^{-1} and symmetric stretch vibrations near 1040 cm^{-1} . The

**Fig. 5.** LC-ESI-MS spectra of (a) 25C-NBOMe in MS mode, (b) 25C-NBOMe in MS/MS mode, and (c) 2C-C in MS/MS mode.

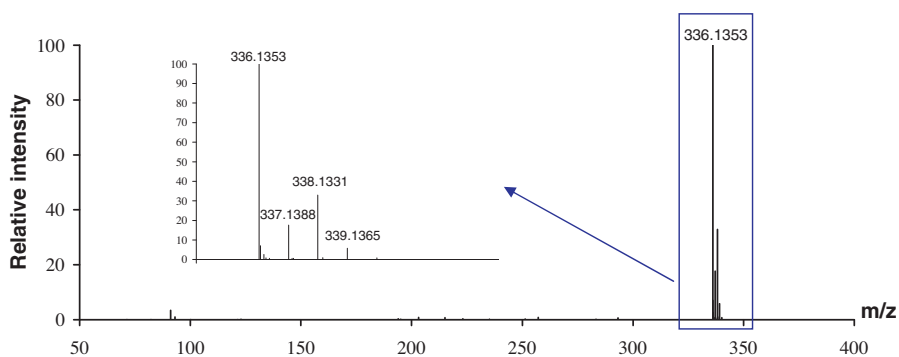


Scheme 2. Proposed fragmentation routes of 25C-NBOMe under ESI.

latter band is characteristic for benzene ring substituted by two methoxy groups located in *para* position as it occurs in the compounds from 25-NBOMe and 2C series. The C–H stretching vibrations characteristic for methoxy groups can also be observed at 2850 cm⁻¹, which additionally confirms that the examined

substance contained aromatic ring combined with methoxy group(s).

The assignment of a band to the halogen–carbon stretching vibrations is not trivial in halogen-substituted aromatic compounds. The presence of a halogen on an aromatic ring can be



m/z	Abundance (% target)		Abundance (% sum)	
	Theoretical	Observed	Theoretical	Observed
336.1361	100.00	100.00	61.58	63.69
337.1394	20.21	17.58	12.45	11.20
338.1338	34.55	32.88	21.28	20.94
339.1367	6.71	5.79	4.13	3.69
340.1393	0.84	0.96	0.51	0.48

Fig. 6. The relative isotopic abundance for the pseudomolecular ion C₁₈H₂₃ClNO₃⁺.

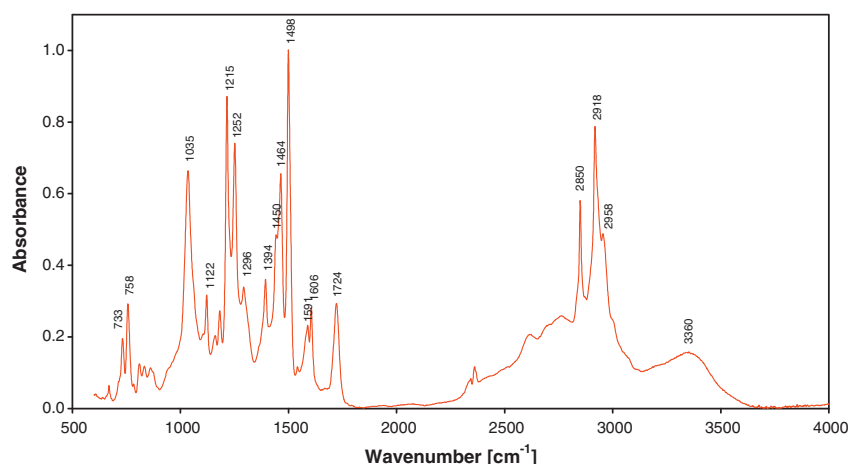


Fig. 7. FTIR spectrum of 25C-NBOMe.

Table 2
NMR assignments for 25C-NBOMe.

Position	δ ^1H (600 MHz)	δ ^{13}C (150 MHz)
1		124.29
1'		119.00
2		151.48
2'		157.70
3	6.81 (s, 1H)	113.18
3'	6.84 (dd, 1H, $J=8.3$; 1.0 Hz)	110.51
4		121.06
4'	7.31 (ddd, 1H, $J=8.3$; 7.5; 1.7 Hz)	131.03
5		149.23
5'	6.94 (ddd, 1H, $J=7.5$; 7.5; 1.0 Hz)	121.43
6	6.89 (s, 1H)	115.75
6'	7.35 (dd, 1H, $J=7.5$; 1.7 Hz)	131.94
CH ₃ -O-(2)	3.62 (s, 3H)	55.92
CH ₃ -O-(2')	3.74 (s, 3H)	55.45
CH ₃ -O-(5)	3.84 (s, 3H)	57.04
Ar-CH ₂ -CH ₂ -NH ₂ ⁺ -	3.12–3.04 (m, 4H)	27.96
Ar-CH ₂ -CH ₂ -NH ₂ ⁺ -		46.92
Ar-CH ₂ -NH ₂ ⁺ -	4.11 (s, 2H)	45.35
>NH ₂ ⁺	8.10 (bs, 2H)	

detected indirectly from its electronic impact on the in-plane C–H bending vibrations, and the first relatively intense band observed at 733 cm⁻¹ can be assigned to chlorine–carbon vibrations.

In turn, the broad band observed at 3360 cm⁻¹ can be assigned to N–H stretch vibrations. In secondary amines one band is observed at 3300–3500 cm⁻¹ (usually 3310–3360 cm⁻¹), while two bands are characteristic for primary amines. The shape and the position of this band confirm that the investigated substance was the secondary amine. The predominant band observed at 1498 cm⁻¹ can be assigned to N–H bending vibrations (secondary amines absorb around 1500 cm⁻¹). Other bands observed in

amines are N–H out-of-plane bending vibrations, which occur around 800 cm⁻¹, and C–N stretchings, which usually occur around 1130–1190 cm⁻¹ (the band with the maximum at 1122 cm⁻¹ can be assigned).

3.5. NMR

Final structure elucidation of 25C-NBOMe was carried out by means of NMR spectroscopy. The signals in the ^1H and ^{13}C spectra were assigned on the basis of one- and two-dimensional homo- and heteronuclear experiments. The full list of signals and appropriate assignments is presented in Table 2.

4. Conclusions

Structure of a new drug from the phenethylamine family has been elucidated. It was found that the blotter papers which have appeared on the Polish drug market in 2011 and 2012 contained *N*-(2-methoxy)benzyl derivative of 2C-C, namely 25C-NBOMe. According to literature data, this substance is a potent partial agonist for the serotonin 2A receptors. Its hallucinogenic action has been reported by users on the Internet fora.

The procedure of 25C-NBOMe identification was based on mass spectrometry, FTIR and NMR spectroscopy. In GC–EI–MS and LC–ESI–QTOF–MS spectra, ions corresponding to 2-methoxybenzyl group attached to the nitrogen atom and those analogous to the parent substance, 2C-C, were observed. Although GC–MS spectrum did not contain molecular ion, derivatization with TFAA reagent made it possible to determine the molecular mass of the investigated substance. The exact mass of the molecule and its chemical formula was confirmed by LC–QTOF–MS experiments and the fragmentation pattern under electrospray ionization was proposed. The bands observed in FTIR spectrum were assigned to characteristic vibrations in 25C-NBOMe molecule. Confirmation of the identity of the investigated substance was performed by ^1H and ^{13}C NMR spectroscopy.

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