Forensic Science International 227 (2013) 7–14

Contents lists available at SciVerse ScienceDirect

Forensic Science International

journal homepage: www.elsevier.com/locate/forsciint

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

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ARTICLE INFO

Article history:
Available online 16 September 2012

Keywords:
Hallucinogen
NBOMe
Legal high
Identification
Blotter papers

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-dimethoxylphenethylamine) 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

☆ This paper is part of the special issue entitled "The 50th Annual Meeting of the International Association of Forensic Toxicologists (TIAFT)". June 3–8, 2012, Hamamatsu, Japan. Guest edited by Adjunct Professor Einosuke Tanaka and Associate Professor Masaru Terada.

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http://dx.doi.org/10.1016/j.forsciint.2012.08.027

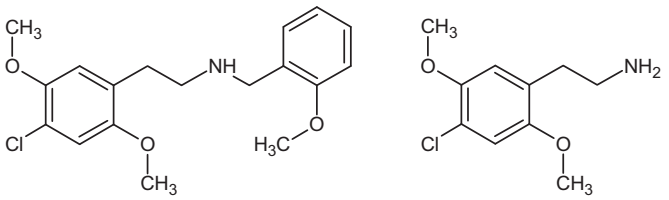

Fig. 1. Chemical structures of 25C-NBOMe and 2C-C.

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) ≥99.9%), formic acid (analytical grade, 89–91%) and TFAA were supplied by Merck (Darmstadt, Germany). Analytical grade ethyl acetate (purity ≥ 99.5%) and chloroform (purity ≥ 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 ($CDCl_3$).

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.

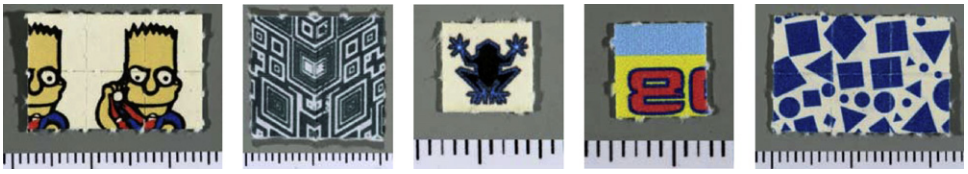

Fig. 2. The blotter papers containing 25C-NBOMe.

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