Research Journal of Forensic Sciences ISSN 2321–1792
Vol. **14(1),** 12-19, January **(2026)** *Res. J. Forensic Sci.*

Case Study

Serendipitous Detection of 3-Chloromethcathinone from Seized Narcotic Drug Samples

Govind S. Bhosle[1], Santosh R. Kote[2]* and Vijay J. Thakare[2]
[1]Regional Forensic Science Laboratory Chhatrapati Sambhajinagar, Home Department, Government of Maharashtra, India
[2]Directorate Forensic Science Laboratory Mumbai, Home Department, Government of Maharashtra, India
santosh.kote27@gmail.com

Available online at: www.isca.in, www.isca.me
Received 10th October 2025, revised 14th November 2025, accepted 23rd December 2025

Abstract

Drug abuse has become concerning issue worldwide, with the illicit drug market continuously evolving to circumvent legal regulations and detection methods. The use of novel psychoactive substances, also known to be "designer drugs" has emerged as a challenge in recent years. Designer drugs are synthesized to mimic the properties of illicit drugs in order to avoid legal restrictions. These designer drugs often contain new and previously unknown chemical compounds, making their identification and detection challenging for law enforcement and forensic laboratories. One such example is the unexpected detection of 3-chloromethcathinone (3-CMC) in narcotic drug samples. In India, the positional isomer of 3-CMC i.e. 4-CMC, is under NDPS act 1985. In the present case work even though the samples were suspected to be Mephedrone, detection of 3-CMC in a narcotic drug sample was achieved successfully by employing various analytical methods such as Thin layer chromatography, UV Spectroscopy, GCMS and H[1] NMR Spectroscopy. The detection of 3-CMC in suspected narcotic drug sample highlights the need for continuous monitoring and analysis of illicit drug samples. It is essential to remain vigilant and adapt detection methods to identify emerging designer drugs, such as 3-CMC.

Keywords: 3-chloromethcathinone, Designer Drugs, GC-MS, [1]H NMR Analysis, New Psychoactive Substances, Positional Isomers.

Introduction

"Designer drugs" are the psychoactive substances synthesized to mimic the physiological properties of known drugs of abuse[1]. Majority of designer drugs are chemically identical to other drugs of abuse but they are altered structurally to avoid legal restrictions. They are often modified structurally in order to get undetectable by conventional drug screening tests. Once a drug is listed in a controlled substance list, chemists in designer drug laboratories quickly change the structure of that drug and create a new substance that isn't listed in controlled substance list. Europe only has reported 265 new psychoactive substances between years 2014 to 2017[2]. It has become major challenge to law enforcement agencies and forensic professionals[3]. The designer drugs also cause a challenge for detection, as it is hard to find a substance by conventional methods in forensic laboratory setup.

One of the most commonly occurring designer drugs are cathinones which have chemical structures based on the 2-phenylethanamine backbone. Basically these, synthetic cathinones are β-keto phenethylamines. There are many synthetic cathinones which falls under international control such as cathinone, methcathinone, cathine and pyrovalerone. 4-methylmethcathinone (4-MMC or 4-methylephedrone) commonly known as Mephedrone, is a synthetic stimulant drug which belongs to the amphetamine and cathinone classes[4]. Manufacturing, possession, selling and consumption of it is banned in many countries and have serious legal implications. Hence drugs seized from the accused are submitted to the forensic science laboratory for identity confirmation. Majority of samples submitted to the forensic laboratories are adulterated with sugars, salts and other low-cost drugs to maximize the profit[5]. Adulteration of these samples makes it even more difficult for detection. Similarly, 3-Chloromethcathinone (3-CMC) is a synthetic derivative of the cathinone family. 3-CMC is one isomeric form of the drug "chloromethcathinone", in which 2-chloromethcathinone (2-CMC) and 4-chloromethcathinone (4-CMC) are the other two positional isomers (Figure-1) currently 3-CMC is not included under international control, but its isomer 4-CMC was placed under international control in 2020[6]. Although 3-CMC was first reported on the drug market in Sweden in October 2014, limited information on 3-CMC is available in the scientific literature.

The distinction of 3-CMC from its positional isomers is done in many, but not all, forensic laboratories. It is probably due to variation in reporting practices across the world. It requires the use of appropriate analytical techniques. Even though 3-CMC and 4-CMC appeared on the drug market at around the same time in 2014, the detection of 3-CMC was remained low in comparison to 4-CMC by law enforcement seizures until 2020.

The significant, increase in seizures of 3-CMC was observed during 2020 and 2021. 3-CMC is being manufactured, imported, distributed, sold, and used as a replacement to 4-CMC in many countries[7].

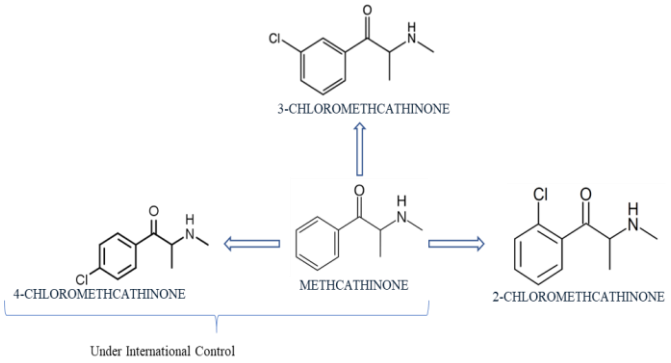


Figure-1: Synthetic Chlorocathinones.

In the present case work detection of 3-Chloromethcathinone in two different narcotic drug samples of different cases (Sample 1 and Sample 2), submitted to the forensic science laboratory was achieved by using advanced analytical methods. Originally the samples of both cases which were submitted at our laboratory were suspected to be Mephedrone (4-Methylmethcathinone).

Materials and Methods

All reagents used in this work were of commercial quality (obtained from Sigma–Aldrich, India or Alfa-Aesar, Heysham, India) and they were used without further purification. Solvents were dried, wherever necessary, using standard procedures. Ultraviolet spectra were obtained using a (model analytikjena Specord S-210 PLUS). Thin-Layer Chromatography (TLC) was carried out on aluminium-backed SiO_2 plates (Merck, Darmstadt, Germany) and spots visualized using ultra-violet light (254 nm) and Dragendroff reagent. GC–MS analysis was performed using an Agilent 8890 GC and Agilent-5977B MSD mass selective detector (MSD) (Agilent Technologies, Wokingham, UK). Proton (H^1) Nuclear magnetic resonance spectroscopy analysis were carried out at Central Instrumentation Facility, Savitribai Phule Pune University, Pune using Bruker Z119470_0152 (500 MHz) instrument.

Preliminary examination: Both the samples (Sample 1 and Sample 2) submitted for detection of Mephedrone were off-white colored crystalline powder. Solubility tests showed that Sample 1 and Sample 2 were soluble in water, methanol and hydrochloric acid. Similarly, the test for chloride as well as sugar was also found positive for both the samples. Presumptive tests such as Cobalt thiocynate test were found to be negative for Sample 1 and Sample 2. The Lieberman test gave yellow coloration and Zimmermann test was also found to be negative for Sample 1 and Sample 2. A microcrystal test using an aqueous extract of Sample 1 and Sample 2 separately and mercuric chloride solution in water did not show paddle wheel and rosette of blade-like crystals under the microscope which are characteristics of microcrystal test of Mephedrone and was found to be negative for the sample in both cases. The results of the Presumptive tests are summarized in Table-1.

Table-1: Colour tests/ spot tests for the sample 1 and Sample 2.

Tests	Test Sample		Ref. Mephedrone
	Sample 1	Sample 2	
Cobalt Thiocynate	No color	No color	Dark Blue color
Liebermann	Yellow color	Yellow color	Dark Yellow color
Zimmermann	Negative	Negative	Negative
Dragendroff	Orange	orange	orange

Thin Layer Chromatography (TLC): Thin-Layer Chromatography (TLC) was carried out on aluminium-backed SiO_2 plates (Merck, Darmstadt, Germany) and spots visualized using ultra-violet light (254 nm) and Draggendroff's reagent. Reference Mephedrone and the suspected Sample 1 and Sample 2 to be tested were spotted on TLC plates with the help of fine capillaries. The plates were developed in a TLC chamber presaturated with a mobile phase. Different solvent systems used in the analysis are presented in Table-2. The plates were then removed, dried in air for 10 min, observed under UV at 254 nm and sprayed with the Dragendroff (DDR) reagent. The Rf values of the spots observed were noted from Figure-2.

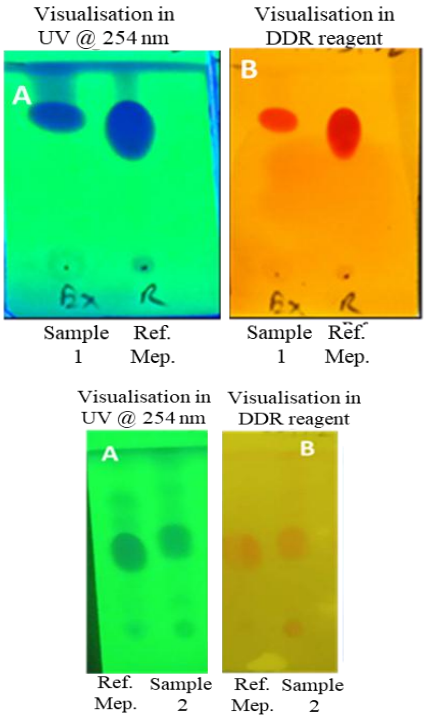


Figure-2: Thin Layer Chromatography of samples in Sample 1 and Sample 2, A) Visualization in UV at 254 nm, B) Visualization in Dragendroff reagent.

Table-2: Rf value data for the Sample 1 and Sample 2.

Solvent System	Ratio	Rf values for Samples		
		Ref. Mephedrone	Sample 1	Sample 2
Ethyl Acetate: Methanol: Ammonia	16:3:1	0.70	0.80	-
Ethyl Acetate: Methanol: Ammonia	17:2:1	0.50	-	0.60

UV Visible spectrophotometry: To corroborate the absence of Mephedrone in Sample 1 and Sample 2, we further analysed these samples by using UV Visible spectrophotometry. The property for instance maximum absorbance (λmax) can be determined with ultraviolet (UV) spectroscopy. This can be important for the characterization and distinction of new psychoactive substances (NPSs). Berger *et al.* used ultraviolet spectroscopy to record the UV-spectra i.e. λmax of 20 different cathinones in a wavelength range of 200 nm-800 nm. They concluded that UV spectroscopy could be used to distinguish between positional benzene ring isomers[8].

Samples under analysis are prepared in 0.1 N HCl and analyzed on UV-Vis spectrophotometer instrument (model Analytikjena Specord S-210 PLUS). A cell of 1 cm path length and a wavelength in the UV range 200-400 nm was used for scanning. The spectra were compared with reference Mephedrone.

Table-3: Maximum absorbance (λmax) of Reference Mephedrone, Sample 1 and Sample 2.

Name of Sample	λ_{max} (nm)
Reference Mephedrone	208, 265
Sample 1	213, 255
Sample 2	213, 255

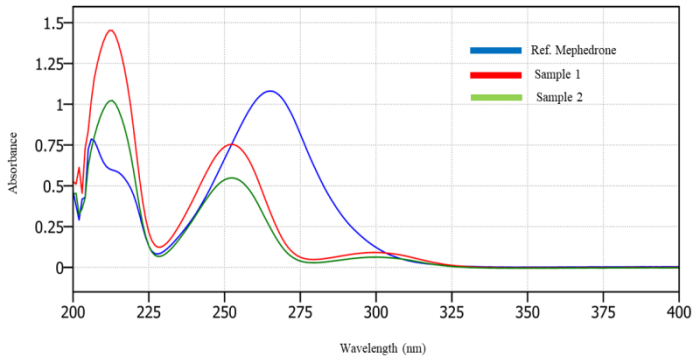


Figure-3: Absorbance spectrum of Reference Mephedrone and Sample 1 and Sample 2 in 0.1 N HCl.

GC MS Analysis: Majority of suspected narcotic drug samples submitted to forensic science laboratories are mixtures of psychoactive substances with cutting agents and other substances such as salts, sugars and other low-cost drugs. GCMS analysis is gold standard in forensic laboratories for routine analysis of such mixtures of psychoactive substances[9].

GC–MS analysis was performed using an Agilent 8890 GC and Agilent-5977B MSD mass selective detector (MSD) (Agilent Technologies, Wokingham, UK) to confirm the absence of Mephedrone in Sample 1 and Sample 2. The energy of 70 eV was used to operate the mass spectrometer in the electron ionization mode. The capillary column (HP5 MS, 30m × 0.25 mm i.d., 0.25m) was used to achieve separation with helium as the carrier gas at a flow rate of 1.5mL min-1. The temperature of the oven were started at 140°C for 1 min, It was then increased to 280°C at a rate of 12.5°C min-1, and then hold at 280°C for 12.5min. A sample of 1µL aliquot of Mephedrone from 1 mg mL−1 in methanol was injected in the split (50:1) mode with a purge time of 1 min. The GC interface and injector temperatures were maintained at 230°C and 280°C respectively[10].

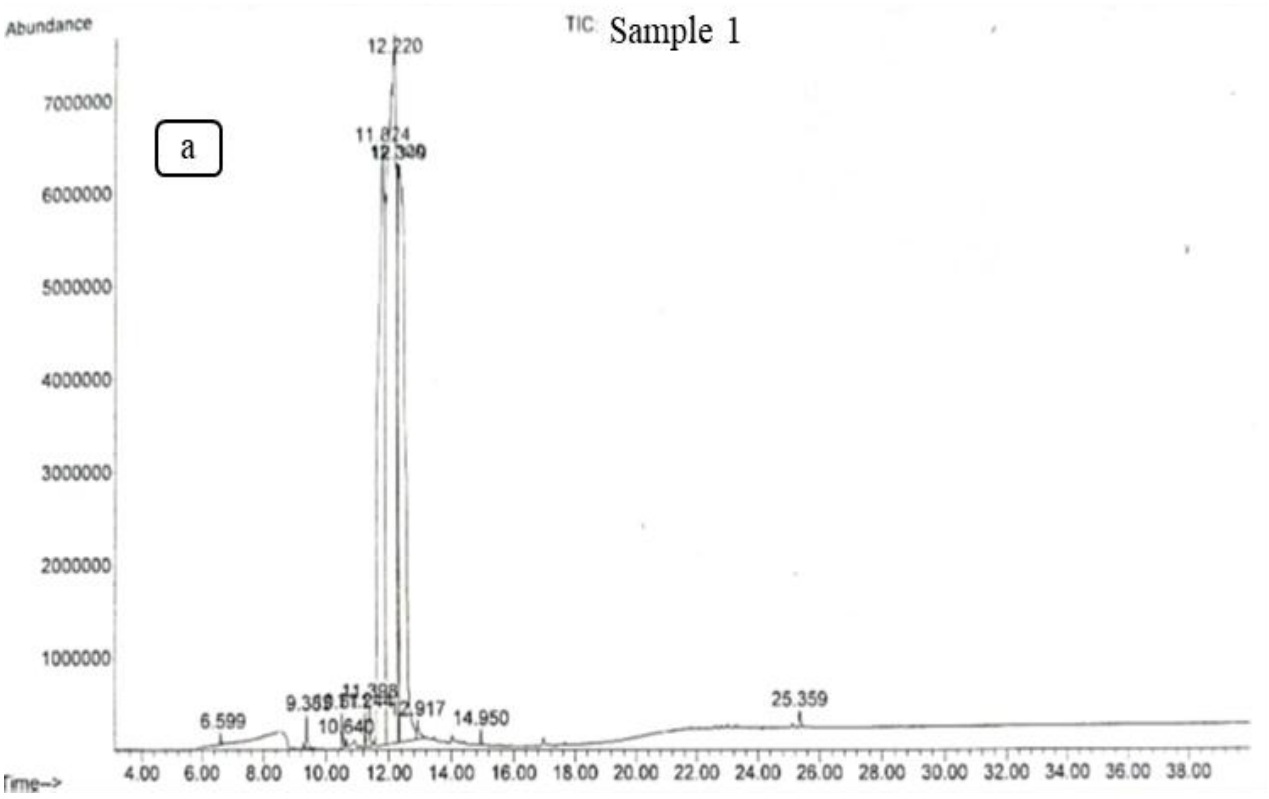
The full scan mode (50–550amu) were used to obtain Mass spectra. Caffeine ranging from 0.001mg mL-1 to 1mg mL-1 prepared in methanol was used as calibration standards.

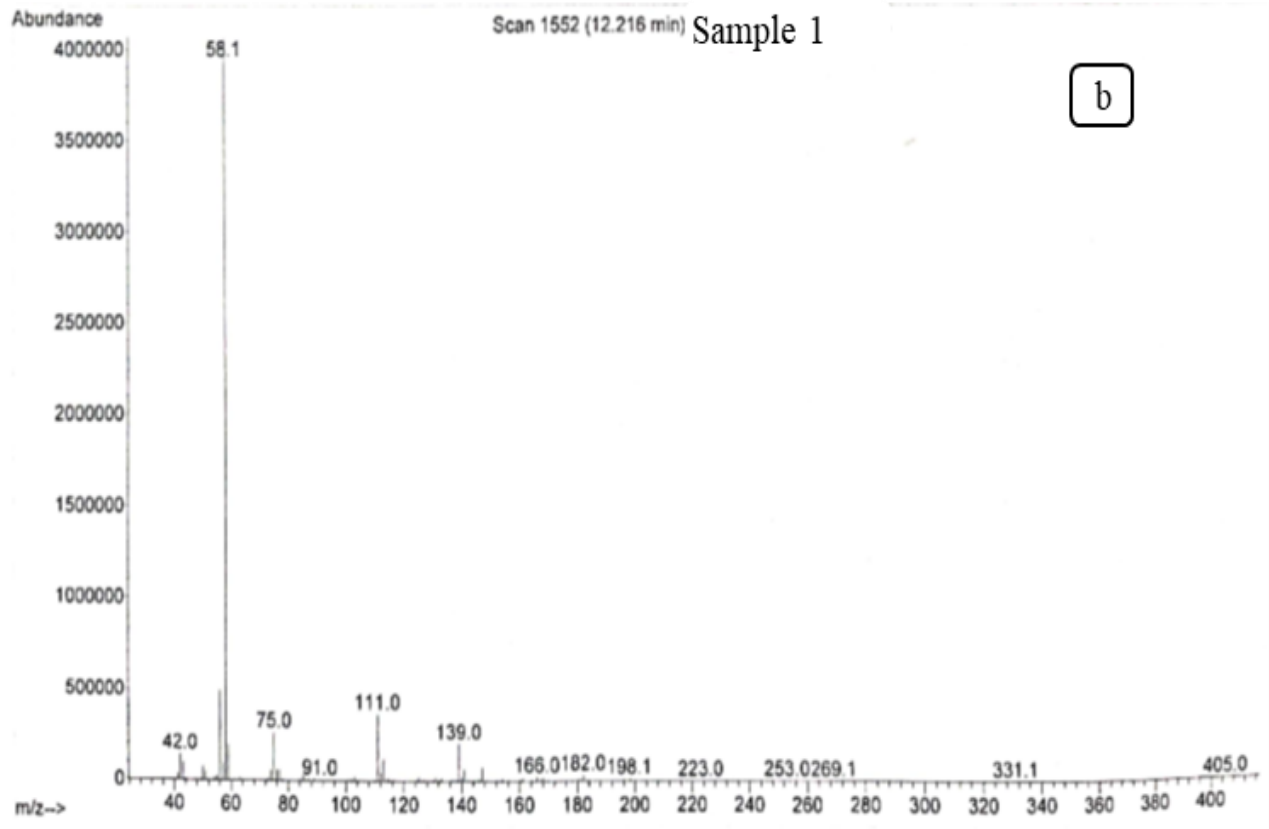
GCMS analysis reveals the presence of Mixture of 3 CMC and 4 CMC in both Sample 1 and Sample 2. Representative GC chromatogram, ESI mass spectrum and Library search hits for Sample 1 are shown in Figure-4. The countries like India where 4 CMC is listed as controlled substance whereas its positional isomer i.e. 3 CMC is not included in the controlled substance act. It becomes imperative to identify exactly which positional isomer is present in the suspected sample 1 and sample 2. Proton (H^1) NMR spectroscopy is ideal technique to differentiate the positional isomers.

Nuclear magnetic resonance (NMR) spectroscopy Analysis: The Bruker Z119470_0152 (500 MHz) instrument was used to record ^{1}H NMR spectra. The ^{1}H NMR spectrum was obtained at room temperature in d6-DMSO as shown in Figure-5. ^{1}H NMR analysis was carried out at Central Instrumentation Facility, Savitribai Phule Pune University Pune. The Chemical Shift (δ) values in ppm and coupling constant in (Hz) for sample 1 and sample 2 are as shown below.

^{1}H NMR Data of Sample 1 (500 MHz, d6-DMSO) δ ppm: 1.45 (d, 3H, *J* = 7 Hz), 2.59 (3H, s), 5.22 (m, 1H, *J*= 7Hz), 7.65 (t, 1H, *J* = 8 Hz), 7.83 (d, 1H, *J* = 8 Hz), 8.00 (d, 1H, *J* =1.5 Hz), 8.08 (t, 1H, *J*= 1.5Hz) and 9.61(s, 1H);

^{1}H NMR Data of Sample 2 (500 MHz, d6-DMSO) δ ppm: 1.44 (d, 3H, *J* = 7 Hz), 2.70 (3H, s), 5.23 (m, 1H, *J*= 7Hz), 7.65 (t, 1H, *J* = 8 Hz), 7.84 (d, 1H, *J* = 8 Hz), 8.01 (d, 1H, *J* =1.5 Hz), 8.08 (t, 1H, *J*= 1.5Hz) and 9.61(s, 1H);


Abundance
TIC: Sample 1
a
12.220
11.824
12.339
6.599
9.389
10.640
12.917
14.950
25.359
Time-->
4.00 6.00 8.00 10.00 12.00 14.00 16.00 18.00 20.00 22.00 24.00 26.00 28.00 30.00 32.00 34.00 36.00 38.00


Abundance
Scan 1552 (12.216 min) Sample 1
b
58.1
111.0
75.0
139.0
42.0
91.0
166.0
182.0
198.1
223.0
253.0
269.1
331.1
405.0
m/z-->
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400

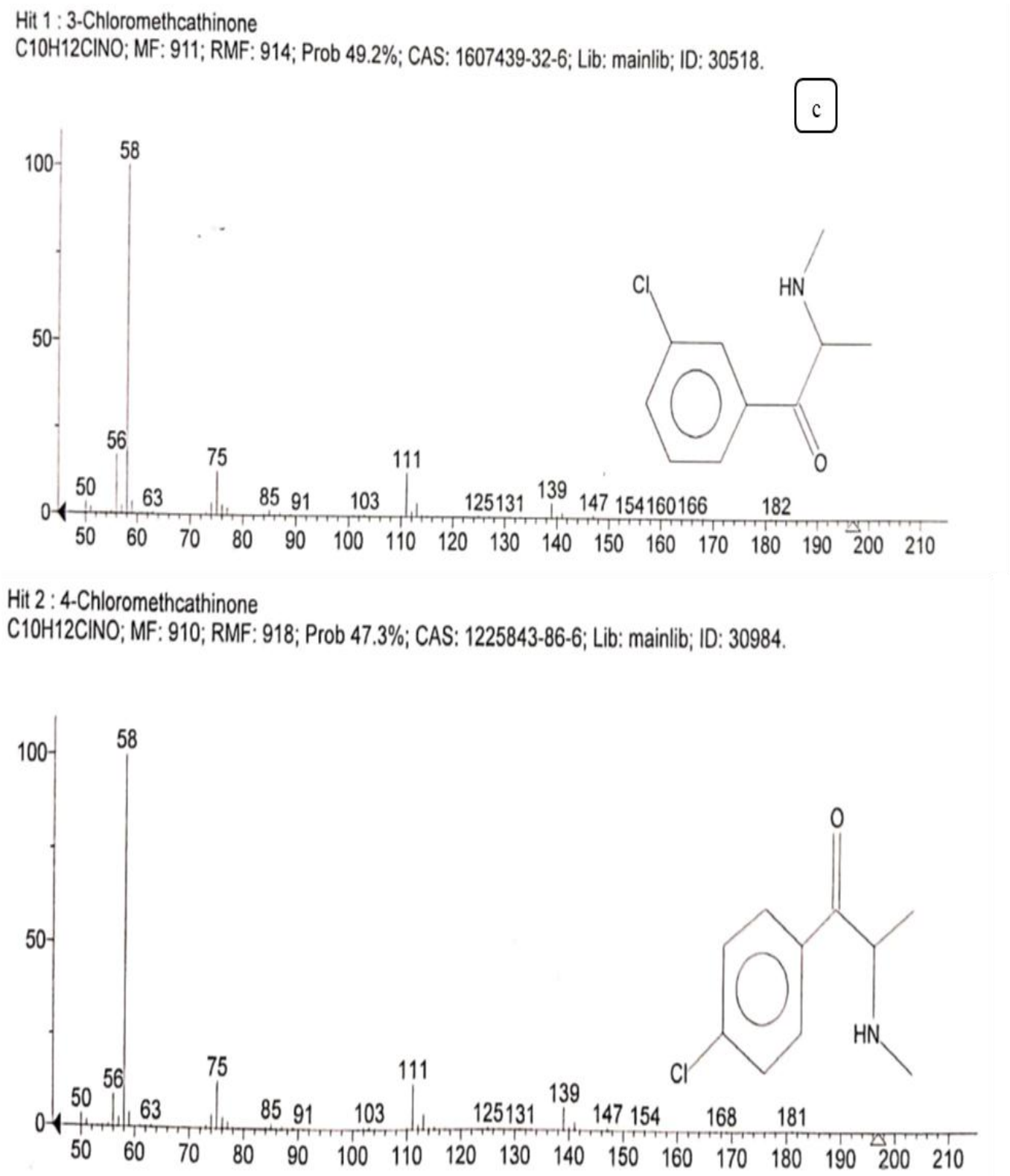


Figure-4: (a) Representative GC chromatogram of sample 1 (b) ESI mass spectrum of sample 1 (c) Library search hits of positional isomers 3-CMC & 4-CMC.

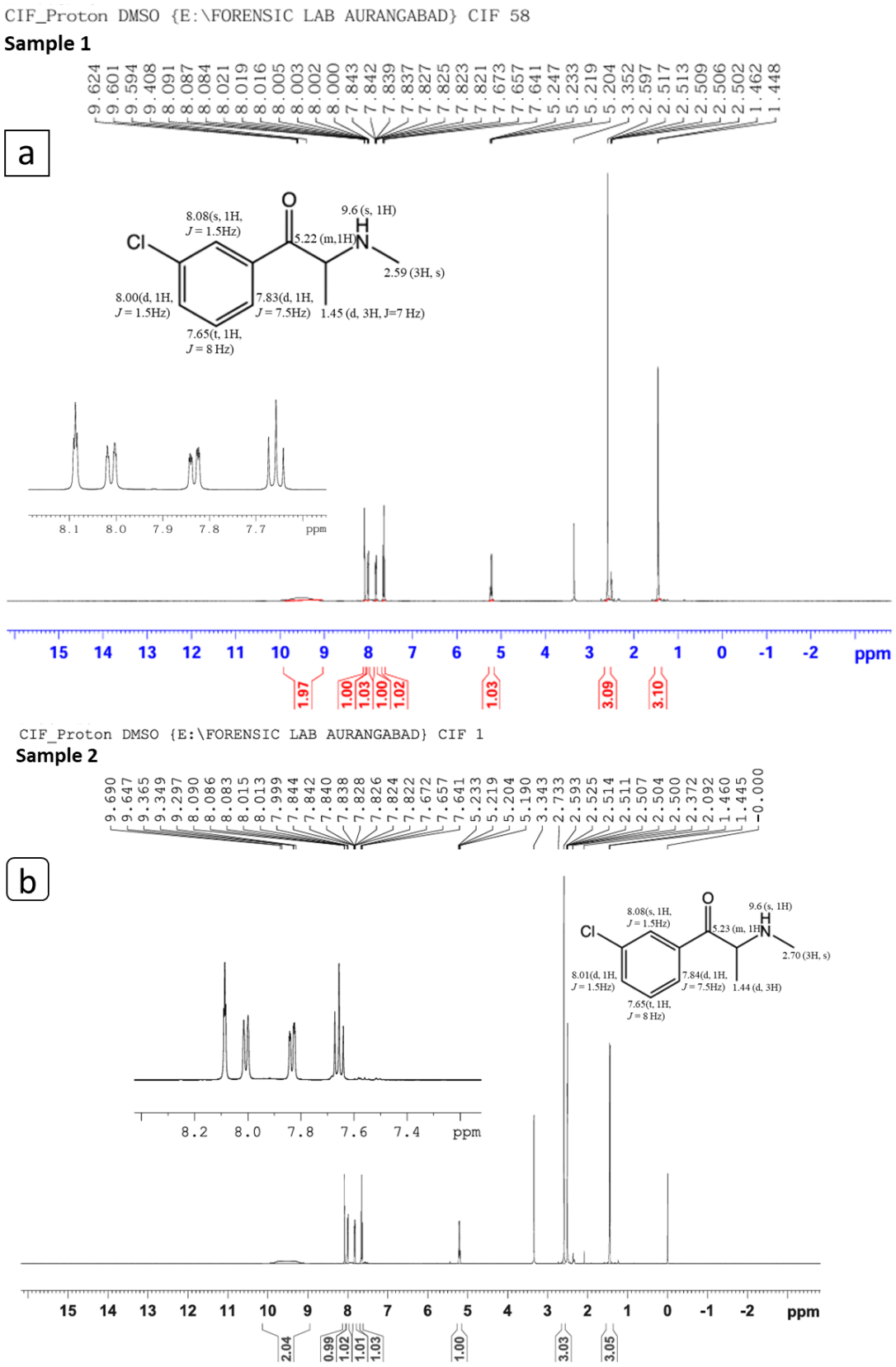


Figure-5: [1]H NMR spectrum (500 MHz, d6-DMSO) of samples in a) Sample 1, b) Sample 2.

Results and Discussion

The Sample 1 and Sample 2 submitted to our laboratory in two different cases were suspected to be Mephedrone. The physical tests such as appearance and solubility tests were carried out routinely. Presumptive tests such as Liebermann and Dragendroff were found to be positive for both Sample 1 and Sample 2 and reference Mephedrone. Zimmermann test was negative for both Sample 1 and Sample 2 and reference Mephedrone. Interestingly Cobalt Thiocynate test was negative for both Sample 1 and Sample 2 but it was positive for reference Mephedrone as usual. The negative result of Cobalt Thiocynate test was indicative of absence of Mephedrone. Since presumptive tests are not conclusive enough for identification of new psychoactive substances (NPSs), advanced analytical methods were used for further analysis.

Thin-Layer Chromatography (TLC) is one of best analytical method for the identification of new psychoactive substances (NPSs) when the reference drug is available. To rule out the presence of Mephedrone in the suspected Sample 1 and Sample 2, Thin-Layer Chromatography was carried out. It was found that Rf values of the reference Mephedrone tallies with the literature reported Rf values. Rf values of Sample 1 and Sample 2 varies slightly as compared to Rf values of the reference Mephedrone as shown in Table-2. This difference in Rf values of reference Mephedrone and both Sample 1, Sample 2 suggest the absence of Mephedrone. This could be attributed to the variations in the interactions of Mephedrone and 3-CMC with the stationary phase of TLC plate.

The findings of TLC analysis were corroborated by recording the absorbance spectrum of reference Mephedrone and Sample 1 and Sample 2 as shown in Figure-3. However, seized NPS samples typically consist of adulterants[11]. UV spectroscopy is unable to differentiate these different substances and cannot provide identification of components of NPS in a mixture. Therefore, a separation method must be used before the detection of the NPS substances with UV spectroscopy. In order to purify the samples, crystallization was carried out by using Hexane and Methanol as solvent. After the standard crystallization protocol off-white crystals of Sample 1 and Sample 2 were obtained and used for all further experiments.

Theoretically the λmax for reference Mephedrone as calculated from Scott's Rules was determined to be 256 nm[12]. The λmax observed for Reference Mephedrone is 265 nm is in agreement with literature reports[13]. The slight bathochromic shift observed could be due to the solvent effect. The Sample 1 and Sample 2 showed similar λmax at 255 nm (Table-3, Figure-3) and are indicative of absence of Mephedrone. This difference in λmax of Mephedrone and the Sample 1 and Sample 2 could be due to (–I) inductive effect and (+M) mesomeric effect of Chloride group present on benzene ring.

GC–MS is the most used technique in narcotics and forensic laboratories because it offers the detection of many substances simultaneously in single analytical method and also saves the time and cost of the analysis. To confirm the absence of Mephedrone and to identify the NPS in the Sample 1 and Sample 2, GC–MS analysis was performed. GCMS analysis did not show the presence of Mephedrone instead it showed presence of both 3-CMC and 4-CMC in Sample 1 and Sample 2. Since 3-CMC & 4-CMC are positional isomers of each other having similar molecular weight which results in to similar retention times on GC and similar mass spectrum. Representative GCMS data has shown in Figure-4. The countries like India it becomes mandatory to precisely identify which positional isomer is present in the seized sample since 4-CMC is regulated as controlled substance but its positional isomers such as 3-CMC and 2-CMC are not listed as controlled substance. It becomes mandatory to use an analytical method which can differentiate the isomers (4-CMC) from isomer (3-CMC).

Since 3-CMC and its positional isomers such as 2-CMC and 4-CMC, have close retention times and identical MS spectra. The general GC-MS methods may not allow distinction between them. Proton (H^1) NMR spectroscopy is a powerful analytical technique for the elucidation of molecular structure. Major advantage of Proton NMR is that it provides identification of NPS isomers and analogues without the need of reference standards. In order to achieve precise identification of positional isomers such as 3-CMC and 4-CMC in the suspected Sample 1 and Sample 2 Proton NMR analysis was carried out.

The observed spectrum showed the presence of characteristic AA'/BB' aromatic system indicating unsymmetrically meta-substituted aromatic system at 7.65 (t, 1H, J = 8 Hz), 7.84 (d, 1H, J = 8 Hz), 8.01 (d, 1H, J = 1.5 Hz), 8.08(t, 1H, J = 1.5Hz). This undoubtedly reveals the presence of 3-CMC in the seized Sample 1 and Sample 2. It also showed deshielded one-hydrogen quartet at 5.22 ppm ($CHCH_3$, J = 7 Hz), a deshielded three-hydrogen singlet at 2.59 ppm ($NHCH_3$), a hightly deshielded broad signal at 9.61 ppm was consistently observed and corresponded to the ammonium salt protons NH singlet (9.61 ppm (s, 1H)) and finally a methyl doublet ($CHCH_3$, 1.45 ppm, J = 7 Hz). The ^{1}H NMR spectrum of Sample 1 and Sample 2 indicated that both these samples were clean with no apparent adulterants or cutting agents. This could be due to the crystallization step carried out prior to ^{1}H NMR analysis.

Conclusion

In the present case work even though the samples were suspected to be Mephedrone, detection of 3-CMC in a narcotic drug sample was achieved successfully by employing various analytical methods such as Thin layer chromatography, UV Spectroscopy, GCMS and H^1 NMR Spectroscopy. The objective of this case study is to provide summary of methods that can be used for the distinguishing and identification of NPS positional isomers in forensic laboratory. It can be envisaged that during routine analysis of samples all methods owns their features,

advantages and drawbacks. Some techniques like H^1 NMR are more discriminatory for NPS positional isomers than others. It is always recommended to use combination of multiple methods for the identification of unknown NPS compound particularly when reference standard is not available.

Acknowledgements

The authors are thankful to Director General (Legal and technical), Directorate of Forensic Science Laboratory, Mumbai, Home Department, Govt. of Maharashtra, for his encouragement and support.

References

1. Airuehia E., Walker L. Y. and Nittler J. (2015). *Journal of Child & Adolescent Substance Abuse*, 24, 186-190.

2. European Drug Report (2017). Trends and Developments, EMCDDA, Lisbon

3. Underwood, E. (2015). #A new drug war.# *Science*, 347, 469-473

4. Manual (2015). #Recommended Methods for the Identification and Analysis of Synthetic Cathinones in Seized Materials.# Manual for use by national drug analysis laboratories United Nations; New York.

5. Prieto A. P. (2019). #Drug adulterant and their effect on user: A critical review, Technical Report.#

6. Abdulrahim D. and Bowden-Jones O. (2015). #Guidance on the management of acute and chronic harms of club drugs and novel psychoactive substances.# Novel Psychoactive Treatment UK Network (NEPTUNE) on behalf of the NEPTUNE Expert Group.

7. Critical review report (2023). #3-Chloromethcathinone.# World Health Organization Expert Committee on Drug Dependence, Forty-sixth Meeting, Geneva.

8. Berger J., Staretz M.E., Wood M., Brettell T. A., (2020) Ultraviolet absorption properties of synthetic cathinones, Forensic Chemistry, 21, 1016-1020

9. Elie M.P., Elie L.E., Baron M.G., (2013). #Keeping pace with NPS releases: fast GC-MS screening of legal high products, Drug Test.# Anal. 5, 281-290.

10. Manual (2020). #Recommended methods for the identification and analysis of synthetic cathinones in seized materials.# Vienna: United Nations Office on Drugs and Crime;

11. Report (2016). #Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG) Recommendations Include: Code of Professional Education and Training Methods of Analysis Quality Assurance United States, Department of Justice Drug Enforcement Administration Executive Office of the President Office of National Drug Control Policy Counter Drug Technology Assessment Center.#

12. Scott A. I. (1964). #Interpretation of the Ultraviolet Spectra of Natural Products.# Pergamon, New York, 1964.

13. Santali E. Y., Cadoganb A. K., Daeidb N. N., Savageb K. A., Sutcliffe O. B., (2011). #Synthesis, full chemical characterization and development of validated methods for the quantification of (±)-4-methylmethcathinone (mephedrone): A new "legal high".# *Journal of Pharmaceutical and Biomedical Analysis*, 56, 246– 255.