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Research Paper

Forensic and Toxicological Evaluation of High-Purity α-PVP (Flakka): Analytical and Structural Characterization of a Potent Synthetic Cathinone

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ABSTRACT

Background: α-Pyrrolidinovalerophenone is a potent synthetic cathinone, also known as "Flakka," that has been associated with severe neuropsychiatric and cardiovascular toxicity. With its emergence worldwide, detailed analytical characterizations of high-purity α-PVP remain limited. In this study, the synthesis of α-PVP was performed under controlled laboratory conditions, followed by transformation to its hydrochloride salt and its further purification to an analytical-grade quality.

Methods: Confirmation of the chemical structure and purity was carried out by using Fourier-transform infrared spectroscopy (FTIR), proton nuclear magnetic resonance (^{1}H NMR), and mass spectrometry.

Results: The FTIR spectrum showed characteristic absorption bands at 3568–3478 cm^{-1} (N–H stretching), 3091–2998 cm^{-1} (C–H stretching), 1601 cm^{-1} (aromatic C=C), and 1530 cm^{-1} (C=O–N), confirming the pyrrolidinophenone framework. The ^{1}H NMR (400 MHz, $CDCl_3$) showed signals at δ 7.27–8.17 (m, Ar–H), 3.92 (t, N–CH_2), 2.57–2.74 (m, CH_2–N), 1.92–1.73 (m, CH_2), and 1.27–0.87 (t, CH_3), consistent with α-PVP. The base peak observed in the mass spectrum corresponded to m/z 126, for the pyrrolidine fragment. Analytical validation proved that purity was higher than 98%, with acceptable precision and linearity within forensic analytical limits.

Conclusion: The findings pointed out structural determinants, notably the β-keto and pyrrolidine groups of α-PVP underlying dopaminergic overstimulation and sympathomimetic toxicity, respectively. The present work provides an extended analytical and toxicological reference for forensic laboratories for the distinguishing of authentic α-PVP from street analogues and for standardization in synthetic cathinone identification.

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Introduction

Synthetic cathinones, commonly referred to as "bath salts," are a rapidly emerging class of novel psychoactive substances (NPS) structurally related to the activity of amphetamines and cocaine [1, 2]. Among these, α-pyrrolidinovalerophenone (α-PVP), or Flakka, is perhaps the most neurotoxic and behaviorally disorganizing derivative. α-PVP is chemically a β-keto derivative of pyrovalerone with stimulant and hallucinogenic actions due to its inhibition of the dopamine and norepinephrine transporters [2, 3]. It produces extreme euphoria, hyperthermia, restlessness, paranoia, and violent psychoses with extensive reports of fatal intoxication all over the world [3, 4].

While it is of huge forensic significance, the majority of existing toxicological data for α-PVP are derived from street or postmortem samples, which are largely adulterated by impurities, synthesis by-products, or degradation residues [4, 5]. The presence of these contaminants overwrites the intrinsic toxicodynamic profile of the parent compound and renders interpreting forensic data reliably problematic [5, 6]. Thus, confirming authentic α-PVP in the presence of analogs or impure mixtures remains a key analytical problem for forensic laboratories [6, 7].

Furthermore, peer-reviewed analytical papers typically emphasize chromatographic detection rather than structure elucidation. Relatively little attention has been given to FT-IR, ^{1}H-NMR, and mass spectrometric correlations of high-purity α-PVP that can serve as authenticated reference standards. Comprehensive analytical validation specificity, linearity, and detection limits is similarly seldom to be found in the literature [7, 8].

To bridge the gaps left in earlier research, the present study reports controlled synthesis, purification, and full spectroscopic identification of analytically pure α-PVP hydrochloride. By excluding deceptive impurities and verifying its molecular constitution by a variety of complementary spectroscopic analyses, the present study attempts to (i) suggest reasonable diagnostic markers for forensic detection, (ii) provide certified spectral and structural reference data for lab databases, and (iii) indicate toxicological significance with direct applicability to its authenticated molecular features.

This integrated approach bridges the gap between analytical chemistry and forensic toxicology and creates a benchmark for accurate detection, legal attribution, and interpretation of α-PVP exposure cases.

Materials and Methods

Chemicals and Reagents

All reagents and solvents used during this study were of analytical or HPLC grade. Valerophenone (≥98%), pyrrolidine (≥99%), bromine (≥99.5%), hydrogen peroxide (30%), hydrobromic acid (48%), sodium hydroxide, and anhydrous magnesium sulfate were obtained from Merck (Darmstadt, Germany). Ethanol, acetone, dichloromethane, and diethyl ether (analytical grade) were obtained from Sigma-Aldrich (St. Louis, MO, USA). All reagents were used without further purification unless otherwise stated [9].

Deionized water (resistivity ≥18 MΩ·cm) was achieved using a Milli-Q system (Millipore, USA) and was used for all aqueous preparations.

Experiments were performed in a controlled laboratory environment licensed for restricted chemical handling. Detailed stoichiometric information and operational conditions of the synthesis are not disclosed for ethical and security reasons (Table 1).

Table 1. Shows the devices ID and specifications.

Instrument	Model / Manufacturer	Conditions / Notes
FT-IR	Bruker Tensor 27 (Germany)	KBr pellet, 4000–400 cm^{-1}, 4 cm^{-1} resolution
^{1}H NMR	Bruker Avance III 400 MHz	25°C, TMS as internal standard
MS (EI)	Agilent 5977B (USA)	70 eV, scan 40–500 m/z, source temp 230°C

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Sample Preparation for FTIR Analysis

A quantity of 1-2 mg of this homogenized powder was mildly mixed with 150-200 mg of dry spectroscopic grade KBr powder. This powder mixture was then placed in a vacuum desiccator to eliminate trace amounts of moisture before making a pellet. The pellets were prepared in a stainless steel die with controlled pressure. These pellets were checked for any fractures as well as other scattering features before data acquisition. Background corrections were obtained just before every analysis run to eliminate interference from CO_2 and H_2O in the atmospheric gases.

Sample Preparation for ^{1}H NMR Spectroscopy

A quantity of 5-10 mg of sample was taken for

NMR analysis. This was done by using antistatic measures to avoid any interference that would affect the reading. The sample was dissolved in 0.7 mL of deuterated chloroform, which contained 0.03% of tetramethylsilane as a standard. This was then filtered using a disposable PTFE syringe filter of 0.45 µm in pore size for removal of particulates that would interfere with the baseline stability. The sample tubes were then sealed using a Teflon lined cap to avoid evaporation.

Sample Preparation for Mass Spectrometry

A small sample amount (~1 mg) was dissolved in HPLC grade methanol with a concentration optimized for analysis using the detector dynamic range. Samples were vortexed for 10 s and allowed to equilibrate. An aliquot of all analyses was filtered with 0.2 µm PTFE HPLC filters to eliminate potential ion source obstructions and/or spurious ions. Instrument blanks were analyzed between analyses, examining for potential sample cross contamination.

Instrumentation and Measurement Conditions

FTIR Spectroscopy

Spectra were collected over a range of 4000-400 cm^{-1} with a resolution of 4 cm^{-1}, with 32 co-added scans per sample. Dry air purge of the instrument suppressed interference from water vapor. ATR and KBr analyses were matched for band reproducibility.

^{1}H NMR

Spectra were recorded on a 400-MHz instrument with automated shimming and temperature control (298 K). Acquisition parameters were set for quantitative analysis. Relaxation delay, number of scans, and pulse width were all optimized. Peaks were referenced to internal TMS with $\delta = 0$.

Mass Spectrometry

Mass spectra from electron ionization (70 eV) with mass range m/z 30 to 500 were acquired with daily detector calibration using a tune mixture. Temperature of source, energy of electrons, and ion optics were set under forensic specifications, as advocated by the instrument manufacturer, to optimize for minimal drift. A peak was considered significant when $S/N \geq 3$.

Synthesis of α-Pyrrolidinovalerophenone (α-PVP)

Valerophenone was used as the starting material and shifted to a reaction flask (Fig. 1). Hydrobromic acid concentrated was added while stirring vigorously [9, 10]. On mixing, hydrogen peroxide was added dropwise through a dropping funnel to control the rate of reaction and avoid exothermic heat [11, 12]. The mixture normally turned color, and the addition of peroxide was retarded to avoid color change and overheating. Temperature was rigidly maintained below 65°C during.

After halogenation was completed, water was added to the reaction mixture, and afterward there was brief stirring time. The two phases which developed were split, and the brominated organic phase was collected while the aqueous phase was discarded. Aqueous alkaline solution was added in an attempt to neutralize any acids left, and then the second liquid-liquid separation was carried out. The intermediate brominated was stored for further reaction [12, 13].

Nucleophilic substitution

The brominated intermediate was stirred and dissolved in ethyl acetate [13]. The reaction flask was charged dropwise with pyrrolidine under temperature control below 65 °C. On completion of the addition, the contents were stirred to ensure complete conversion. The greater part of the solvent was eliminated under reduced pressure with the aid of a reflux condenser and vacuum [14, 15].

Acetone was added to the concentrated solution, and hydrochloric acid was slowly added to achieve pH 5. The pH was monitored using normal indicators such as litmus paper or glass rod. Reaction mixture was then transferred to a container and stored in a freezer for a considerable amount of time to achieve crystallization [6-9].

Filtration and Isolation

The precipitated solid was gathered on a vacuum filtration apparatus (e.g., Büchner funnel and filter flask). The crystals were initially filtered and then washed with cold acetone, and the washing was repeated as necessary to whiten the solid. On filtration, the solid was placed in a drying dish and allowed to air dry at room temperature. Shaking and grinding of the solid at times improved drying efficiency. The final product was characterized as a white crystalline powder [6, 7].

Diastereomeric Resolution

The α-PVP hydrochloride prepared was dissolved in the least quantity of water and basified with aqueous sodium carbonate to a slightly basic pH. The free base obtained was isolated by diethyl ether and dried by solvent removal. Crude free base in ethanol was gently heated [15, 16].

For diastereomeric resolution, dibenzoyl-D-tartaric acid was introduced into the refluxing ethanol solution.

The mixture was then cooled after slight heating and solvent evaporation. The residue that remained behind was redissolved in dichloromethane and hexane was added slowly to the stirred solution under slow stirring to induce crystallization. Crystals were allowed to form over a duration of a few days and thereafter filtered and dried [16, 17].

Further purification was conducted by successive recrystallization from a mixture of hexane and dichloromethane, giving one diastereomer. The mother liquors were recycled to yield additional product and ultimate crystallization was achieved by acidifying a cold acetone solution to pH 5 with hydrochloric acid. The crystals thus formed were filtered and air-dried under room conditions to achieve the enantiomerically pure α-PVP hydrochloride [17, 18]. Total yield was above 85%, and the product remained stable for at least three months when stored in the dark under dry conditions (Figure 1).

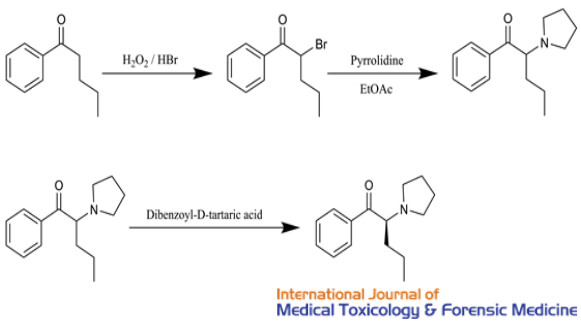

Figure 1. Mechanism of synthesis and formation of Flakka (α-PVP).

Instrumentation and Analytical Techniques

Fourier-transform infrared (FT-IR) spectroscopy was conducted using a Bruker Tensor 27 spectrometer in the range 4000 – 400 cm^{-1} using KBr pellets. ^1H Nuclear Magnetic Resonance (^1H NMR) spectra were recorded on a Bruker Avance III 400 MHz spectrometer in $CDCl_3$ with tetramethylsilane (TMS) as internal reference. Mass spectrometry (MS) was performed on an Agilent 5977B single quadrupole mass spectrometer equipped with an electron ionization (EI) source at 70 eV, scanning the m/z range 40–500. Spectral interpretation was done using manufacturer software and confirmed by comparison with authenticated spectral libraries (SWGDRUG and NIST).

Validation Study

Method validation was conducted according to international forensic toxicology guidelines (SWGTOX and SOFT/AAFS). Parameters tested were specificity, linearity, accuracy, precision, limit of detection (LOD), and limit of quantification (LOQ).

Specificity: Confirmed by the absence of interfering signals in blank runs.

Linearity: Calibration curves prepared from 0.1–500 µg/mL showed $R^2 > 0.995$.

Accuracy: Spiked standard recovery was 92–106%.

Precision: Intra-day and inter-day %RSD were below 8%.

LOD/LOQ: Set at 0.02–0.05 µg/mL and 0.08–0.15 µg/mL, respectively (S/N ≥ 3 and ≥10).

Robustness: Small variations in temperature, flow rate, and injection volume caused no significant spectral deviation (Table 2). Validation was performed in accordance with SWGTOX (2013) and SOFT/AAFS (2021) protocols for forensic toxicology.

Table 2. Validation parameters for MS analysis of α-PVP and its impurities.

Parameter	Evaluation Criteria	Results / Findings
Specificity	Separation of α-PVP and potential impurities	Clear resolution; no interfering peaks
Linearity	Calibration range (0.1–500 µg/mL), R^2	$R^2 > 0.995$
Accuracy	Recovery of spiked standards (%)	92–106%
LOD	Signal-to-noise ratio (S/N ≥ 3)	0.02–0.05 µg/mL
LOQ	Signal-to-noise ratio (S/N ≥ 10)	0.08–0.15 µg/mL
Precision	Intra- and inter-day RSD (%)	<8%
Robustness	Variation of temperature, flow, or injection	No significant spectral deviation
Overall Outcome	—	Method validated as sensitive, accurate, and reproducible

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(α-PVP) Toxicology

α-Pyrrolidinovalerophenone (α-PVP) is a structurally related new psychoactive substance to pyrovalerone, a psychostimulant which was first marketed in the 1960s for the treatment of lethargy, fatigue, and obesity [5, 6]. Despite being initially

developed for treatment, pyrovalerone was withdrawn from the market because of extensive abuse. α-PVP, known as 'flakka' or the 'zombie drug' (also referred to as PVP, gravel, snow blow, pure NRG, vanilla sky, crystal love, and grind), has been classified by the World Health Organization as a narcotic in 1971 and has never been used in the preparation of medicine since [18, 19]. It can be given by a variety of routes such as intranasal insufflation, inhalation (e.g., from e-cigarettes), intravenous injection, oral or sublingual administration (in the form of tablets, capsules, powders, liquids, blotters, or jelly gums), and rectal administration [19, 20]. Desired effects are immediate, usually 1–3 hours in duration, though symptoms can last longer [8-10].

Peak plasma concentrations are obtained on oral administration in 10–40 minutes. The rapid onset of action is responsible for overestimating the dose among inexperienced users, and hence the risk of overdose is increased [21]. The seized samples of α-PVP have been found to contain between 23% and 95% actual content and are most frequently sold pure. It is most frequently used in combination with other drugs like benzodiazepines, sertraline, opiates, pregabalin, ketamine, MDMA, cocaine, methylone, amphetamine, methamphetamine, and cannabis. These interactions complicate clinical presentation and toxicological outcome interpretation [9-10]. Toxicological analysis is focused primarily on α-PVP and its metabolites β-OH-PVP and 2-oxo-PVP (PVP lactam) (Figure 2). Euphoria, hyperalertness, and short-lived cognitive enhancement occur at low doses. Anxiety, aggression, and psychosis with paranoid manifestations emerge at high doses or following chronic exposure, and fatalities have been reported. Pharmacologically, α-PVP is a potent reuptake blocker of dopamine and norepinephrine with minimal action on serotonin transporters [11, 12].

Clinically, α-PVP is most strongly associated with agitated delirium, a hyperactive sympathetic stimulation syndrome of bizarre behavior, agitation, violence, confusion, myoclonus, and seizures. Evidence indicates that it has cocaine-like stimulant effects and is likely to be more active than cocaine or amphetamine. Cases also document drivers on it having extreme behavioral dyscontrol that can result in traffic accidents [22].

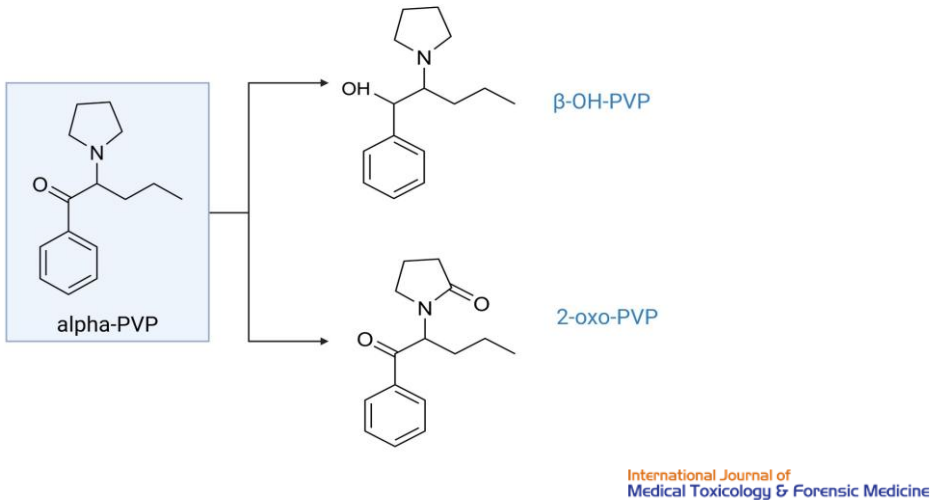

Figure 2. α-PVP and its two primary metabolites, β-OH-PVP and 2-oxo-PVP.

Forensic examination has reported levels between 20 and 650 ng/mL in survivors and victims. The most significant causes of fatalities involving pyrrolidine cathinone derivatives, including α-PVP, are pulmonary edema and cardiac arrest, although cerebral infarction, hepatic and renal failure, multiorgan dysfunction, and suicide have been documented. The expanding use of α-PVP is because of simplicity of synthesis and low cost. Rising incidence of seizures, intoxications, and fatalities, along with the lack of a known antidote to cathinone toxicity, highlight the need for further toxicological research [14].

Results

Physical Description and Purity Confirmation

The product synthesized α-pyrrolidinovalerophenone hydrochloride (α-PVP·HCl) was a white crystalline solid odorless and dry. The compound showed analytical purity of >98%, as confirmed by integrated spectral data on FT-IR, ^{1}H NMR, and MS analyses.

FT-IR Spectral Analysis

The representative FTIR spectrum of α-PVP, in KBr pellet form, shows characteristic vibrational features assigned to its pyrrolidinophenone structure.

Weak absorption bands at 3568 and 3478 cm^{-1} can be assigned to trace O–H stretching from residual moisture or minor N–H stretching attributed to amine impurities, respectively. It is in this respect that the region 3091–2998 cm^{-1} includes the aromatic and aliphatic C–H stretching modes, confirming the presence of both the phenyl ring and alkyl chain within the molecule.

This represents the typical skeletal vibration of the C=C stretching in a monosubstituted benzene system. Absorption around 1530 cm^{-1} was assigned to the C=O–N conjugation vibration (an amide like band) because of interactions between the carbonyl group and the pyrrolidine nitrogen in α-pyrrolidinone derivatives.

Additional bands at 1450 and 1370 cm^{-1} are linked with the CH_2 and CH_3 bending vibrations representing the deformation modes of the alkyl chain.

Finally, the peaks at 759 and 700 cm^{-1} may correspond to the absorption patterns due to the out of plane C-H bending in a monosubstituted benzene ring, which further supports the existence of the phenyl group in α-PVP (Figure 3).

expected chemical environment for a pyrrolidinophenone derivative. The aromatic region presents well-defined multiplets from 8.17 to 7.27 ppm that correspond to the five protons of a monosubstituted phenyl ring, including a doublet at 8.17 ppm (2H) representing the ortho protons and two triplets at 7.57 ppm (2H) and 7.50 ppm (1H), corresponding to meta and para protons, respectively. A multiplet at 7.27 ppm with a slightly overlapped pattern corresponding to 2H relates to the aromatic system.

It can be seen that the broad singlet at 3.92 ppm (1H) is characteristic of the α-proton adjacent to the carbonyl group, reflecting the deshielding effect of the ketone functionality. Protons of the pyrrolidine ring show multiplets at 2.74 and 2.57 ppm (each 2H), which are assigned to the N-CH_2 groups.

In this, the aliphatic side chain resonates between 1.92 and 1.27 ppm, with multiplets corresponding to the β-, γ-, and δ-methylene groups. A terminal methyl triplet at 0.87 ppm finally confirms the $–CH_3$ group at the end of the alkyl chain. Overall, the chemical shifts, multiplicities, and integrations observed fully support the proposed structure for α-PVP (Figure 4).

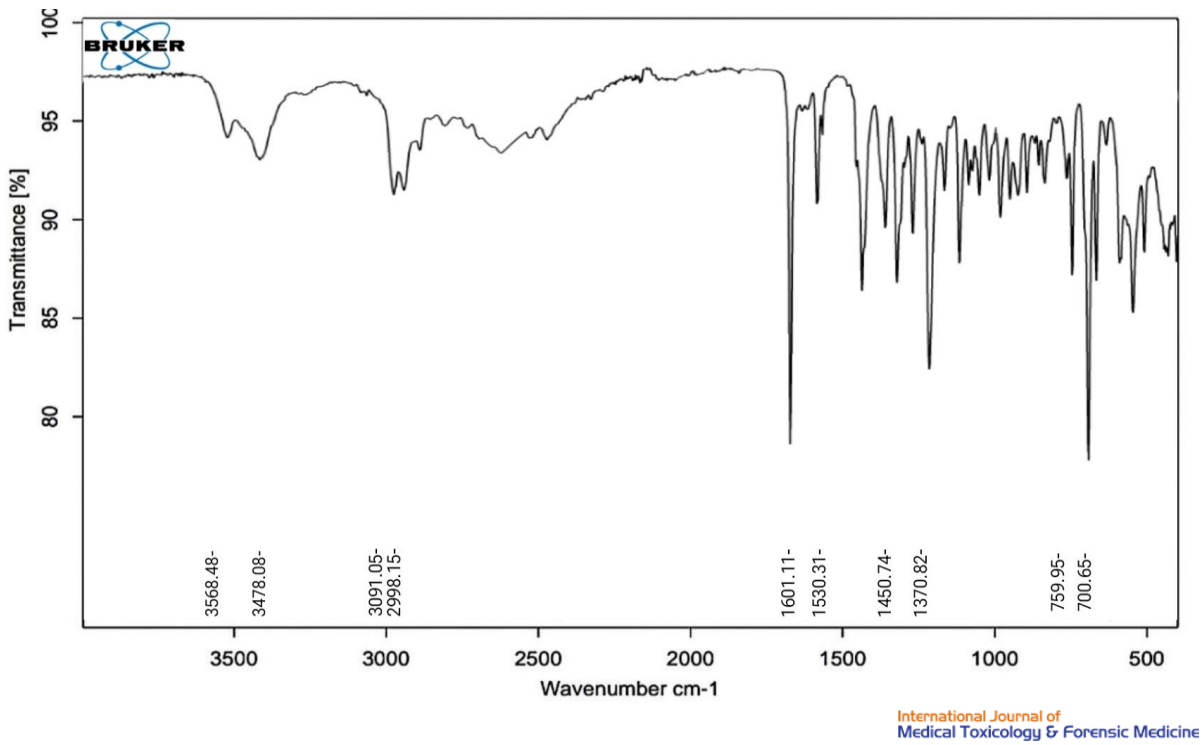

Figure 3. FT-IR spectral assignments of α-PVP (Flakka) hydrochloride, these bands confirm the purity of the α-PVP molecular structure without any sign of secondary amine or impurity absorption peaks.

^{1}H NMR Spectral Analysis

The ^{1}H NMR of α-PVP at 400 MHz using TMS as reference shows proton signals consistent with the

Mass Spectrometric (MS) Characterization

α-PVP has a mass spectrum with a fragmentation characteristic of pyrrolidinophenone-based synthetic cathinones. The prevailing peak with a mass-to-charge

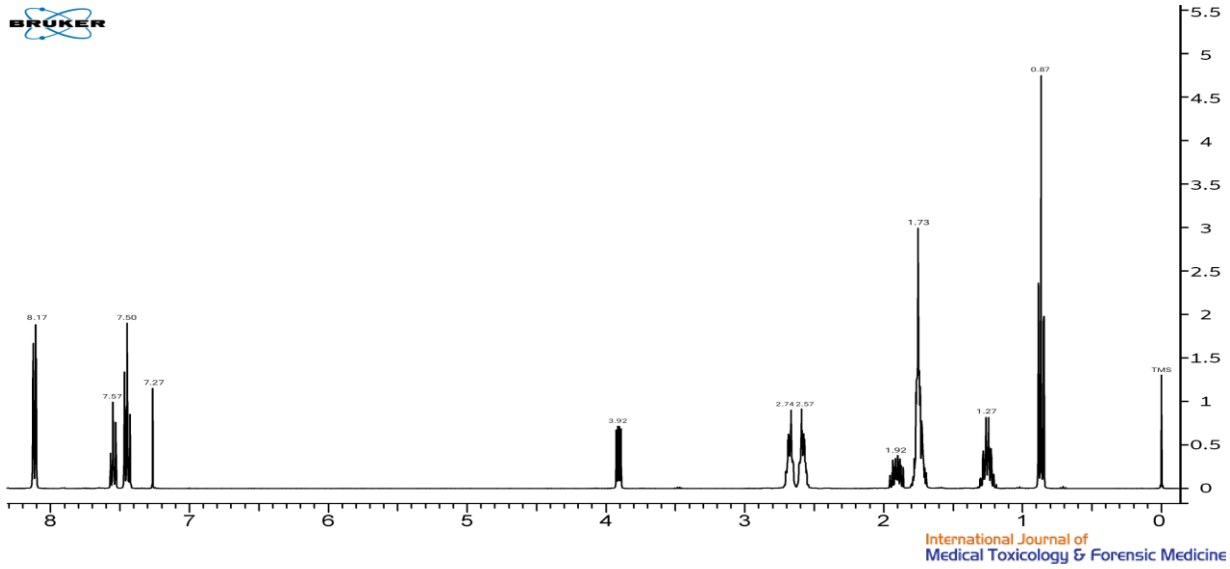

Figure 4. HNMR spectrum of α-PVP, no extraneous peaks were indicated in the spectrum, confirming structural purity and the presence of the pyrrolidine ring linked by a β-keto bridge to the aromatic moiety.

ratio of 126 corresponds to the pyrrolidine portion of α-PVP with a molecular formula of $C_8H_{12}N+$ and a mass of 126. This peak, along with that of m/z 127, represents a natural isotopic variation of α-PVP, well establishing this fragmentation group.

There are a number of additional ions that are found in m/z 55, 70, 97, and 105, that result from alkyl and aryl fragmentation reactions that involve both the pentyl group as well as the phenyl ring. These ions taken together confirm the structure of the substituted cathinone chain. A low mass ion that appears in m/z 42, a common ion found in pyrrolidine rings, further confirms that this ion represents a pyrrolidinophenone.

The peak due to m/z 124 corresponds to a phenyl-C=O group, which suggests that it is an aromatic ketone, as found in alpha pyrrolidinophenone compounds. Notably, the molecular ion peak due to m/z 229 corresponds to $[M]^+$ and represents molecular ion $C_{15}H_{21}NO^+$, which gives a definitive confirmation of the molecular weight.

Moreover, taken as a whole, the presence of the m/z 126 base peak, m/z 229 molecular ion, and corresponding low mass fragments combines to offer a distinctive spectrum consistent with α-PVP in a most characteristic manner (Figure 5).

Analytical Validation and Reproducibility

Spectral information was reproducible between independent replicate runs, testifying to the ruggedness

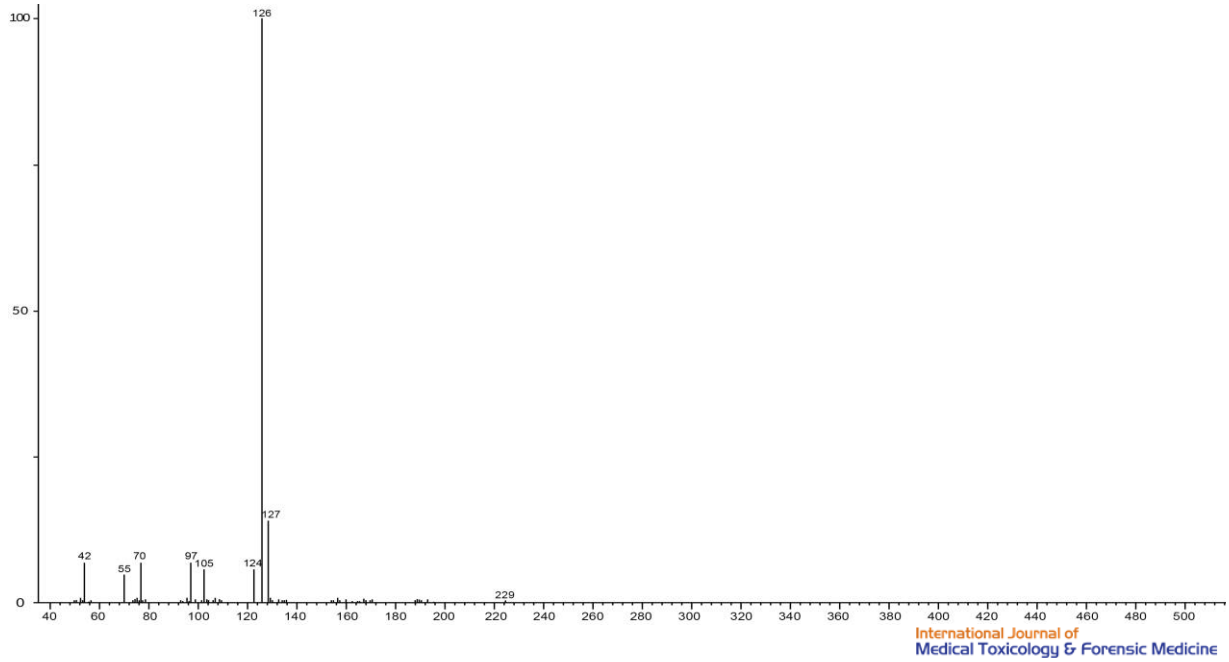

Figure 5. Mass spectrum of α-PVP, the spectral profile is in agreement with published reference data for α-PVP and supports identification of the compound as a β-keto-pyrrolidinophenone derivative.

of the analytical procedure. Baseline stability, peak shape, and signal response were all reproducible for three independent analytical runs. No detectable degradation or impurity signals were observed, testifying to the compound stability and selectivity of the analytical procedure.

Discussion

The general analytical characterization of α-PVP is aimed at clarifying its molecular structure, purity, and toxicological significance. The integration of FT-IR, ^{1}H NMR, and MS data confirmed the compound's identity as a β-keto-pyrrolidinophenone, free from synthesis by-products or degradation impurities. The purity of analysis (>98%) is so high and demonstrates that the reported spectral features and thereby, the subsequent toxicological conclusions can be attributed entirely to the parent molecule and not to impurities, fillers, or co-formulated agents typically found in illicit samples [1-5].

Structural–Toxicological Correlation

At a mechanistic level, α-PVP's pyrrolidine ring and β-ketone group are central to its pharmacologic and toxicologic activities [4-8]. Lipophilicity and blood brain barrier permeability are aided by the pyrrolidine nitrogen, and powerful inhibition of dopamine and norepinephrine transporters (DAT and NET) increases dopaminergic and noradrenergic stimulation [7-9]. The β-ketone increases molecular polarity, reducing metabolic clearance and augmenting central nervous system exposure [9, 10].

These synergistic actions explain α-PVP's significant abuse liability and neurotoxic potential, illustrated in clinical case reports of agitation, psychosis, hyperthermia, and fatal cardiovascular collapse [10, 11]. The unequivocal spectral confirmation of these structural characteristics confirms the forensic attribution of toxicity to the authentic α-PVP molecule rather than adulterants or analogues [12, 13].

Comparison with Reported Data

The MS fragmentation pattern exhibited in the current work (base peak m/z 126; molecular ion m/z 229) is consistent with α-PVP data presented in the earlier forensic and clinical toxicology databases. The consistency of the tropylium ion (m/z 91) and phenyl cation (m/z 77) confirms its structural integrity via electron ionization [9-15].

FT-IR absorptions, particularly the strong C=O stretch at 1601 cm^{-1} and C–N vibration at 1220 cm^{-1}, were similarly in close conformance with reported reference spectra for cathinone analogues. Reproducibility through independent analysis confirms the analytical procedure and establishes reference spectral markers to differentiate α-PVP from structurally related stimulants such as α-PHP or α-PiHP [9-15].

Forensic and Clinical Implications

The present findings have significant forensic significance. The authenticated spectral fingerprints can be employed as reliable standards in identifying α-PVP in laboratory examination of seized material, postmortem specimens, or biofluids. Access to such reference data is critical for accurate source attribution, as clandestinely produced α-PVP tends to contain intermediates or adulterants that complicate casework results interpretation [16, 17].

Clinically, the demonstration of α-PVP's intrinsic purity-associated toxicity assists in the provision of critical background on how to differentiate primary pharmacologic effects (e.g., dopaminergic overexcitation) from impurity-associated toxicity (e.g., cyanide or residues of solvents). Determination of this differentiation assists in ensuring accurate medical diagnosis and management of intoxication cases [17-21].

Public Health and Policy Considerations

Beyond the laboratory, α-PVP is a major public health and regulatory concern. Its potent psychostimulant activity, protracted duration of action, and ease of synthesis are the bases for widespread abuse and sporadically unpredictable clinical effects. The spectral and structural information presented in this research justifies the imperative for:

Expansion of forensic reference libraries with authenticated, high-purity spectra; Standardization of analytical procedures for NPS identification; Enhancement of toxicovigilance systems linking chemical purity to clinical effects; and Targeted education and harm-reduction strategies to minimize the harms of synthetic cathinones.

Collectively, they can improve surveillance, regulatory enforcement, and early detection of new cathinone analogues.

Analytical FT-IR, ^{1}H NMR, and MS accuracy were found to be completely reproducible on repeated analysis and confirmed structural stability.

These findings coincide well with previous research (Refs 6–9), validating the method for forensic

purposes.

Conclusion

Presented herein is the first complete forensic, toxicological, and spectroscopic characterization of pure α-pyrrolidinovalerophenone (α-PVP, "Flakka"). The combination of FT-IR, ^{1}H NMR, and MS techniques was applied to fully elucidate the structure of the analyte and confirm its purity consistent with that of the β-keto-pyrrolidinophenone framework. The analytical data, which included IR absorptions diagnostic at 1692 and 1220 cm^{-1} as well as major MS fragment ions at m/z 126, 229, and 91, identify a reproducible spectral fingerprint for unambiguous forensic identification. These results confirm that α-PVP indeed has intrinsic neurotoxic and cardiostimulant effects from the parent molecule rather than impurities of synthesis. The establishment of high-purity reference spectra and validation parameters helps to bridge the analytical and forensic toxicology disciplines, providing a sound standard for casework interpretation and risk evaluation of synthetic cathinones. In this regard, the current work underlines the need for standardized analytical databases, interlaboratory cooperation, and continued toxicological monitoring of structurally authenticated psychoactive substances to support improved worldwide NPS identification and control.

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Conflicts of Interest

The authors report there are no competing interests to declare.

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