

## CASE REPORT

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### *Datura stramonium*: A Fatal Poisoning

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**ABSTRACT:** A case report of death caused by ingestion of *Datura stramonium*, also referred to as jimsonweed, thorn apple, or Jamestown weed, is presented. Mass spectral data on urine extracts of a 20-year-old male showed the molecular ions and principal fragment ions of scopolamine and atropine, present in *Datura stramonium*.

**KEYWORDS:** toxicology, poisons, *Datura stramonium*, mass spectrometry, tropane alkaloids, scopolamine

Through the years, numerous case reports of tropane alkaloid poisonings have appeared in the medical literature [1-10]. However, with the exception of cocaine overdose, very little confirmatory analytical data concerning tropanes in biological specimens of blood, urine, and other media are available [11]. In this report, we describe a fatal poisoning from *Datura stramonium* (also referred to as jimsonweed or Jamestown weed and thorn apple) and the analytical sequence used to confirm the presence of tropane alkaloids in the urine of the deceased.

#### Poisoning by *Datura stramonium*

The chief biochemical constituents of *Datura stramonium* are hyoscyamine and scopolamine. Hyoscyamine, or more specifically *l*-hyoscyamine, occurs in colorless crystalline needles and is levorotatory. Extraction from the vegetable material results in racemization with conversion to the *d,l*-compound atropine. Hyoscyamine is extremely toxic, and the chief manifestations of hyoscyamine poisoning are dilated pupils, impaired vision, dryness of the skin and mucous membranes, extreme thirst, and hallucination followed by loss of consciousness. The catch phrase used by emergency room doctors to remember the cardinal symptoms of atropine poisoning is "Blind as a bat, mad as a hatter, and red as a beet."

Historically, *Datura stramonium* was grown in England in the 16th century, apparently from seeds obtained from the Middle East. Early settlers near Jamestown, VA, were familiar

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with stramonium as a pot herb and cultivated the plant from seeds brought with them. This link with the Jamestown colony established the common name of Jamestown weed, which was subsequently modified in certain areas to jimsonweed. *Datura stramonium* grows wild in the United States today and is also referred to as thorn apple, devil's apple, and angel tulip. The potent pharmacologic effects of the compounds present in stramonium have been known for centuries, with many references to the toxic properties of atropine-containing plants made in early nonscientific literature such as Homer's *Odyssey* and Shakespeare's *Romeo and Juliet*. In *Antony and Cleopatra*, Shakespeare writes that the plant was employed by Cleopatra in her wooing of Caesar.

#### Case History

A 20-year-old male, who lived on a ranch, was an amateur herbist. On returning home from one of his herb-gathering trips, the subject brewed a pot of tea for himself and several friends from some of the vegetable material he had gathered. After ingesting the tea, they all complained of double vision and extreme dryness of the throat and began to hallucinate. The 20-year-old died shortly thereafter. His friends were admitted to the hospital with dilated pupils and dry flushed skin. A quantity of vegetable material from which the tea was made was brought to the hospital. Examination of the vegetable material showed leaves, flowers, and fruit characteristic of *Datura stramonium*. Stramonium [12] usually occurs in irregular matted masses (Fig. 1). Figure 2 shows the white trumpet-shaped flower, which is 15.24 to 20.32 cm (6 to 8 in.) in length. The immature fruit (Fig. 3) is somewhat conical, four-valved, and covered with short stiff thorns and contains numerous seeds.

#### Summary of Autopsy Findings

On gross examination, multiple petechiae were seen in the epicardium and similar hemorrhages were found throughout the endocardium in the right ventricle. The lungs showed



FIG. 1—*Datura stramonium*. Bush is 60 to 90 cm (2 to 3 ft) in diameter and approximately 45 cm (18 in.) high and contains numerous white trumpet-shaped flowers.



FIG. 2.—Close-up view of trumpet-shaped flower of *Datura stramonium*.



FIG. 3.—Immature fruit of *Datura stramonium*.

severe hyperemia and edema. Subcapsular petechiae were seen in the liver. The brain weighed 1600 g and was hyperemic and edematous.

Microscopic examination of the lungs revealed diffuse edema and focal hemorrhages within the alveolar lumens. The heart showed well-preserved myocardial fibers and was negative histologically except for scattered epicardial and endocardial hemorrhages. Microscopically, the brain showed evidence of hyperemia and edema but no other significant effects. The appearance of the remaining organs was not remarkable.

When the body was initially examined at the scene of death, it was found to be in full rigor and marked by posterior lividity. External examination of the body produced no remarkable findings except that the pupils were unequal in size, with the right measuring 4 mm in diameter and the left measuring 2 mm. The teeth were tightly clenched, and some partially dried blood was seen within the external nares. Regurgitated gastric material was found within the mouth, but there was no definite obstruction of the airway at the level of the larynx and below.

## Experimental Procedure

At the time the mass spectra used in this study were obtained, a double-focusing mass spectrometer (Du Pont 21-491) operating in the electron impact mode was used. The ionizing potential was 250 to 300  $\mu\text{A}$ ; the accelerating potential was 1100 V coupled with an electric sector voltage of 100 V. To perform the analysis, a portion of the urine extract was added to a glass capillary tube, the solvent evaporated, and the tube introduced into the mass spectrometer using the direct insertion probe. The temperature of the ion source was 175°C. As the temperature of the probe tip was adjusted from 80 to 195°C, mass spectra were recorded on a recording oscillograph (CEC 5-124A) at a chart speed of 25 mm/s (1 in./s). Peak assignment was made by using a digital mass marker (Du Pont) that had been calibrated over the perfluorokerosene range. Spectra at a probe tip temperature of 140 to 150°C gave the best abundances for the fragment ions used for identification.

Postmortem specimens were analyzed for the presence of free hyoscyamine and scopolamine. Conjugated forms were not included in this analysis. Both hyoscyamine and scopolamine are basic alkaloids that can be extracted, isolated, and concentrated by acid-base partitioning with diethyl ether or chloroform. Analyses of the extracts by ultraviolet spectrophotometry and gas and thin-layer chromatography were either negative or inconclusive.

## Results and Discussion

Mass spectral analysis of the extracts revealed the presence of characteristic mass to charge ratio ( $m/z$ ) peaks. At the high mass range, molecular ions of scopolamine ( $m/z$  303) and hyoscyamine ( $m/z$  289) were evident. Characteristic peaks at  $m/z$  285 and 271, signifying loss of water from the parent ions of scopolamine and hyoscyamine, respectively, were also present. Both parent species contain hydroxyl groups beta to a phenyl ring, facilitating loss of water under electron impact. Loss of water to yield the olefin can occur through fragmentation or thermal modes. Here, loss of water is due primarily to fragmentation, as evidenced by the absence of both molecular ions at low probe temperatures, that is, 90°C.

Two base peaks are also of importance: one at  $m/z$  94, which represents a scopolamine ion, and one at  $m/z$  124, which represents an ion of hyoscyamine. These fragment ions exhibited significant abundances in the extract:  $m/z$  94, relative abundance (RA) of 56% and  $m/z$  124, RA of 49%. The  $m/z$  94 and 124 fragments were the second and third most abundant fragments in the mass spectrum. The most abundant peak was at  $m/z$  83. This was undoubtedly due to an impurity that came off at the same probe temperature as scopolamine and hyoscyamine. Other indications that impurities were present were the  $m/z$  285, 271, and 256 fragment ions, commonly observed in spectra of biological specimens. Since the Du Pont instrument used to analyze the samples was not interfaced to a gas chromatograph to achieve separation of the components, it was not surprising to observe interfering fragment ions.

Recently, an HP 5985 GC/MS/DS (Hewlett-Packard, Inc.) was installed in the laboratory. Since the urine and urine extracts were no longer available, an attempt was made to analyze the Du Pont mass spectral data with various programs of the HP system. First, a known sample of scopolamine was injected into a 0.91-m (3-ft) packed column (2% OV-101) and the spectrum recorded. A molecular ion at  $m/z$  303 was observed, as it was when the urine extract had been analyzed on the Du Pont spectrometer. The known scopolamine sample was also analyzed using the direct insertion probe mode of the HP 5985 instrument. The spectrum was the same as that recorded by gas chromatography-mass spectrometry.

The observed spectrum was compared with spectra in the condensed National Bureau of Standards Library Data Bank. There were two matches; the first gave a 98.10% correlation with scopolamine. It is interesting to note that neither the condensed nor the full library scan listed a molecular ion for scopolamine. All the  $m/z$  abundances of the peaks from the original spectrum obtained by the Du Pont instrument were measured and entered into the "syn-

URINE SAMPLE, SCOPOLAMINE & HYOSCYAMINE  
TABULATED DATA FROM DUPONT 21-491 MASS S. 1 SCANS ( 1 SCANS, .02 MINS)  
# 1 1.0  
MASS RANGE: 26.0, 305.0 TOTAL ABUND= 3771.

SCAN #

# 1 RET. TIME: .00 TOT ABUND= 3766. BASE PK/ABUND: 83.0/ 270.

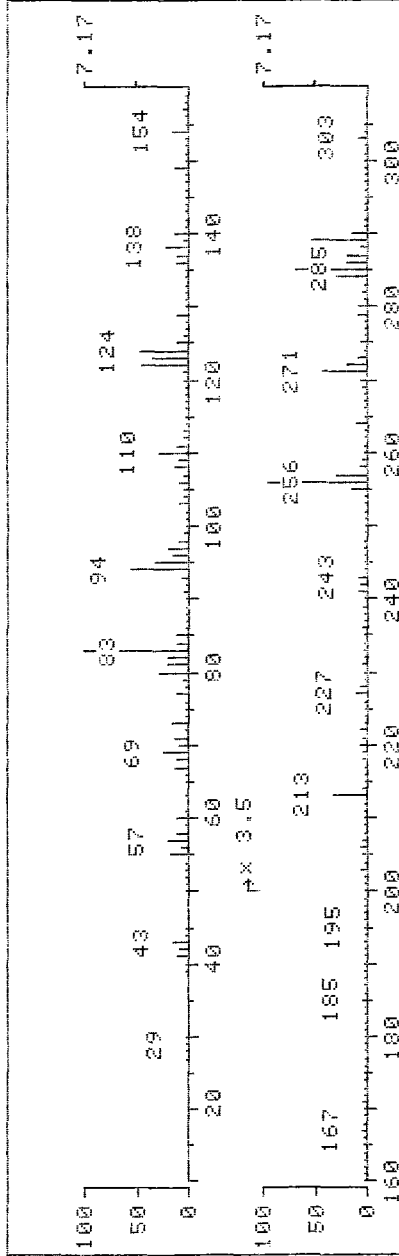


FIG. 4—HP 5985 GC/MS/DS synthesized mass spectrum from data of the Du Pont 41-491 system. Direct insertion probe 140 to 150°C.

thesize" program of the HP 5985 data system. This synthesized mass spectrum (Fig. 4) was subjected to a library search. Note that a scale expansion factor of 3.5 was used for the mass range 200 to 310. The results of the library searches are shown in Figs. 5 and 6. Using 303 as the molecular weight range, a correlation of 87.23% (best match) was obtained for scopolamine. Likewise, using 289 as the molecular weight range, a correlation of 73.46% (best match) was found for hyoscyamine. These correlations, although low because of the presence of abundant fragments from impurities, suggest that the death described in this report resulted from ingestion of *Datura stramonium*.

## Conclusion

The investigation at the scene, physical and analytical identification of the consumed vegetable matter, and analytical toxicological confirmation of the presence of scopolamine and hyoscyamine in the urine of the deceased suggest that death was due to *Datura stramonium* poisoning.

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REF.    SPECT #= 1 LSN= 1. MW= 0 FRN=5020
        265 PEAKS, 176 SIGNIFICANT MAX K 19.7

LIBRARY 3000 38 SPECTRA SEARCHED, 3 HIT(S)

.8723 Benzeneacetic acid, .alpha.-(hydroxymethyl)-,9-methyl-3-oxa
      -9-azatricyclo[3.3.1.02,4]non-7-yl ester, [7(S)-(1.alpha.,2.
      beta.,4.beta.,5.alpha.,7
      SPEC= 2004 LSN= 22496. MW= 303 C17H21NO4. . .SCOPOLAMINE
      FRN = 3014 [NBS 22498.] CAS # 0000051343 EPA # 0000014480
      MATCHING PEAKS CONTAMINATED MISSING PEAKS QUAL INDEX = 674
      13.8 9 12% 1.6 1 2% .0 0 0% MULTIPLIER = .37

.7460 + Androstan-3-amine, N-ethyl-, (3.beta.,5.alpha.)-(9CI)
      SPEC= 2024 LSN= 22516. MW= 303 C21H37N
      FRN = 3014 [NBS 22518.] CAS # 0055320462 EPA # 0000048160
      MATCHING PEAKS CONTAMINATED MISSING PEAKS QUAL INDEX= 674
      12.0 8 7% 1.6 1 2% 2.0 1 6% MULTIPLIER= .95

.5649 + Carbamic acid, diphenyl-, p-tolyl ester (8CI)
      SPEC= 2014 LSN= 22506. MW= 303 C20H17NO2
      FRN = 3014 [NBS 22508.] CAS # 0010369978 EPA # 0000014474
      MATCHING PEAKS CONTAMINATED MISSING PEAKS QUAL INDEX=238
      9.3 7 2% .0 0 0% 6.3 3 8% MULTIPLIER=.71
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FIG. 5—Library search of molecular weight range 303.

REF. SPECT # = 1 LSN = 1 MW = 0 FRN = 5020  
 265 PEAKS, 176 SIGNIFICANT MAX K 19.7

LIBRARY 3000 49 SPECTRA SEARCHED, 3 HIT(S)

.7346 + Benzeneacetic acid, .alpha.-(hydroxymethyl)-, 8-methyl-8-aza bicyclo[3.2.1]oct-3-yl ester, [3(S)-endo]- (9CI)  
 SPEC = 942 LSN = 21434. MW = 289 C17H23NO3. . HYOSCYAMINE  
 FRN = 3014 [NBS 21436.] CAS # 0000101315 EPA # 0000042342  
 MATCHING PEAKS CONTAMINATED MISSING PEAKS QUAL INDEX = 728  
 12.6 8 11% 1.8 1 5% 2.2 1 8% MULTIPLIER = 1.61

.7259 1H-Pyrazole-1-carboximidamide, 4,5-dihydro-3-methyl-4-[(4-nitrophenyl)hydrazono]-5-oxo- (9CI)  
 SPEC = 918 LSN = 21410. MW = 289 C11H11N7O3  
 FRN = 3014 [NBS 21412.] CAS # 0042541264 EPA # 0000029809  
 MATCHING PEAKS CONTAMINATED MISSING PEAKS QUAL INDEX = 299  
 12.8 8 6% .0 0 0% 4.3 2 5% MULTIPLIER = .56

.6129 + Carbamic acid, diphenyl-, phenyl ester (8CI)  
 SPEC = 951 LSN = 21443. MW = 289 C19H15NO2  
 FRN = 3014 [NBS 21445.] CAS # 0005416455 EPA # 0000013904  
 MATCHING PEAKS CONTAMINATED MISSING PEAKS QUAL INDEX = 529  
 10.8 7 9% .0 0 0% 6.1 3 7% MULTIPLIER = .46

FIG. 6—Library search of molecular weight range 289.

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