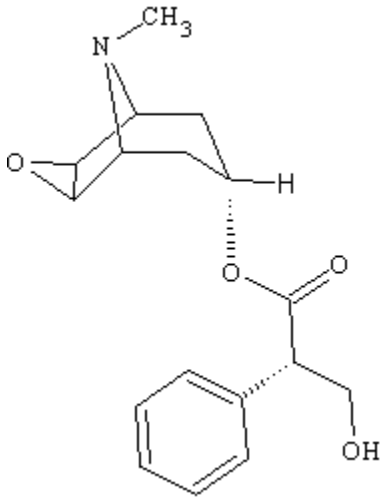
SCOPOLAMINE

Latest Revision: August 15, 2005



1. SYNONYMS

CAS #:

Base: 51-34-3
Hydrobromide: 114-49-8

Other Names:

(α*S*)-α-(Hydroxymethyl)benzeneacetic acid (1α,2β,4β,5α,7β)-9-methyl-3-oxa-9-azatricyclo[3.3.1.$0^{2,4}$]non-7-yl ester

6β,7β-Epoxy-1α*H*,5α*H*-tropan-3α-ol (-)-tropate; 6β,7β-epoxy-3α-tropanyl *S*-(-)-tropate

6,7-Epoxytropine tropate
Scopine tropate
Tropic acid ester with scopine
Hyoscine
l-Scopolamine

2. CHEMICAL AND PHYSICAL DATA

2.1. CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{17}H_{21}NO_4$	303.4	59
Hydrobromide	$C_{17}H_{21}NO_4 \cdot HBr \cdot 3H_2O$	438.3	195
Hydrochloride	$C_{17}H_{21}NO_4 \cdot HCl$	339.8	200
Methylnitrate	$C_{17}H_{21}NO_4 \cdot CH_3NO_3$	380.4	***

2.2. SOLUBILITY

Form	A	C	E	H	M	W
Base	FS	FS	FS	FS	FS	(Hot) FS
Hydrobromide	SS	SS	I	I	FS	FS
Hydrochloride	SS	SS	I	I	FS	FS
Methylnitrate	***	I	I	I	SS	FS

A = acetone, C = chloroform, E = ether, H = hexane, M = methanol and W = water, VS = very soluble, FS = freely soluble, S = soluble, PS = sparingly soluble, SS = slightly soluble, VSS = very slightly soluble and I = insoluble

3. SCREENING TECHNIQUES

3.1. COLOR TESTS

REAGENT	COLOR PRODUCED
Liebermann	Red orange
Wagner	Brown to black

3.2. CRYSTAL TESTS

REAGENT	CRYSTALS FORMED
Gold chloride in Acetic Acid	Hydrobromide: clusters of rods and blades Hydrochloride: long thin spear-shaped crystals

3.3. GAS CHROMATOGRAPHY

Method SCO-GCS1

Instrument: Gas Chromatograph operated in split mode with FID

Column: DB-1, 30 m x 0.25 mm x 0.25 μm film thickness

Carrier gas: Hydrogen at 1.3 mL/min

Make-Up gas: Nitrogen at 40.0 mL/min

Temperatures: Injector: 230°C
Detector: 280°C
Oven Program:
1) 150°C initial temperature 2 min
2) Ramp to 190°C at 5°C/min
3) Hold final temperature for 1.0 min

Injection Parameters: Split Ratio = 20:1, 1µL injected

COMPOUND	RRT	COMPOUND	RRT	COMPOUND	RRT
methylbenzylamine	0.09	methyl paraben	0.21	caffeine	0.50
P2P	0.10	penicillin	0.21	antipyrine	0.54
amphetamine	0.11	salicylamide	0.21	benzphetamine	0.55
nicotinic acid	0.11	phenmetrazine	0.22	diphenhydramine	0.58
phentermine	0.11	MDA	0.23	aminopyrine	0.61
methamphetamine	0.12	MDP2P	0.23	doxylamine	0.62
ethylamphetamine	0.13	phendimetrazine	0.23	palmitic acid	0.66
fenfluramine	0.13	MDMA	0.27	phthalic acid	0.66
dimethylamphetamine	0.14	aminorex	0.28	dipyrone	0.68
safrole	0.15	methyl aminorex	0.28	eicosane	0.72
salicylic acid	0.15	MDEA	0.30	procaine	0.72
cathine	0.16	ibuprofen	0.33	dextromethorphan	0.84
methcathinone	0.16	hexadecane	0.34	strychnine	0.85
PPA	0.16	MBDB	0.34	phenyl-2-napthylene	0.88
nicotinamide	0.17	guaifenesin	0.35	hyoscyamine	0.89
chloroephedrine	0.18	acetaminophen	0.36	atropine	0.89
chlorpheniramine	0.18	MMDA	0.37	amitriptyline	0.90
ephedrine	0.18	phenacetin	0.38	**scopolamine**	**1.00 (9.1 min)**
pseudoephedrine	0.18	chloromdma	0.40	tetracosane	1.07
butylamphetamine	0.21	methylphenidate	0.44	chlordiazepoxide	1.16
				quinine	1.41

4. SEPARATION TECHNIQUES

Scopolamine can be separated from the tablet, powder, or plant matrix by solvent extraction.

5. QUANTITATIVE PROCEDURES

N/A

6. QUALITATIVE DATA

See spectra on the following pages for Mass Spectrometry, FT-IR, Vapor Phase IR, FT-Raman, and Nuclear Magnetic Resonance.

7. REFERENCES

Budavari, S., *The Merck Index, 13th Edition*, Merck and Co., Inc., 2001.

Churchill, K.T., "Angel Trumpet," *Microgram* 1995; 28(8):250.

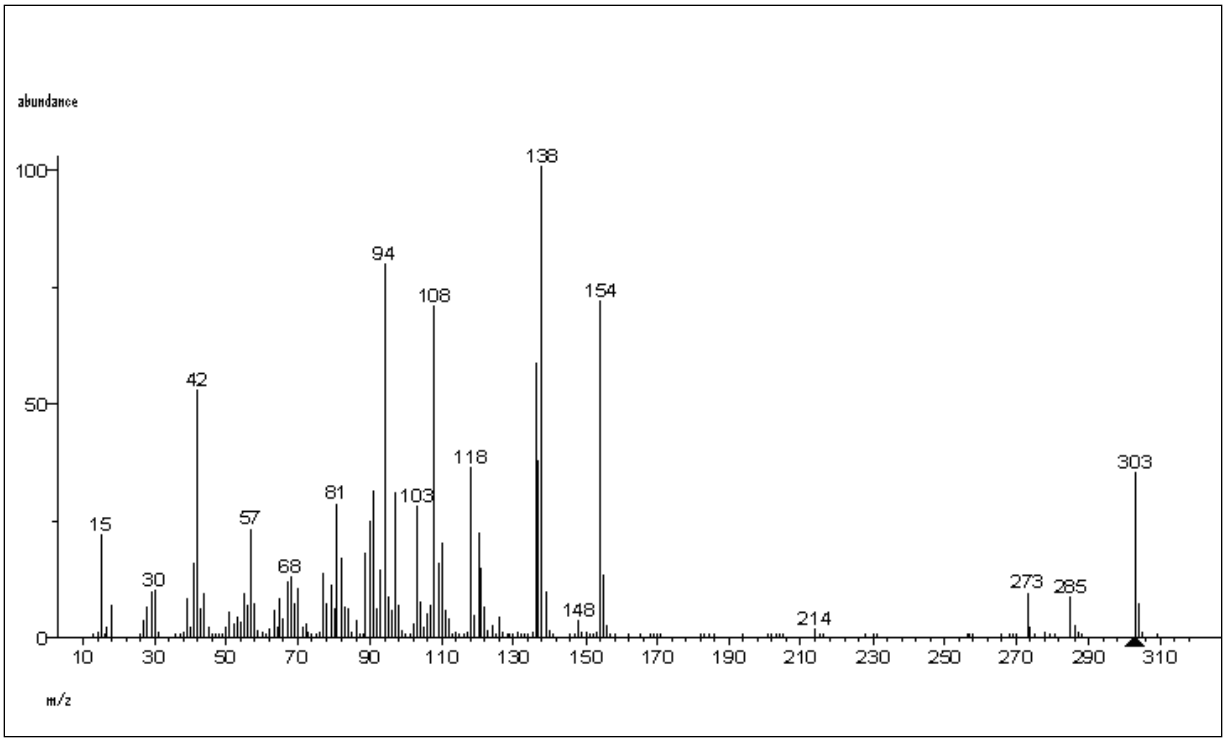
Koverman, Gary, "Identification of Scopolamine and Hyoscyamine in Jimson Weed (*Datura stramonium*)," Microgram 1993, 26(6):19.

Swiatko, Jamie, *et al*., "Further Spot Tests and Microcrystal Tests for Identification of Cocaine," J. Forensic Sciences, Vol. 48, No. 3, May 2003.

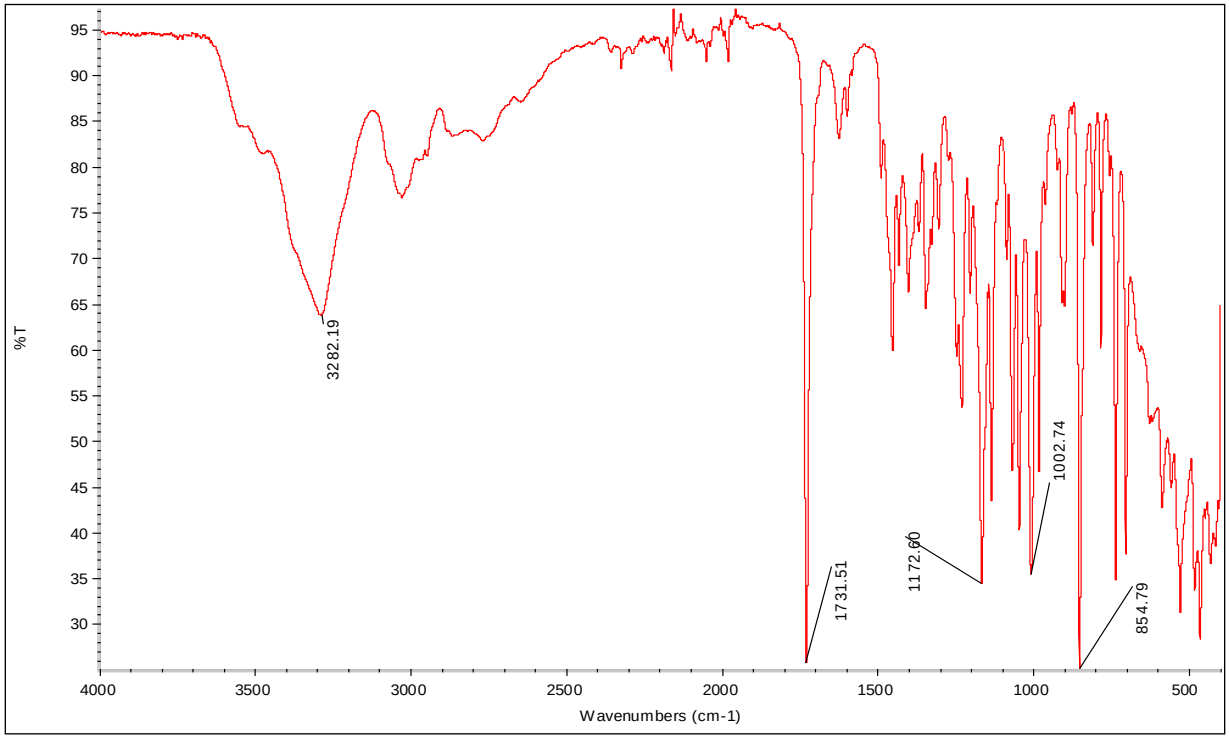
8. ADDITIONAL RESOURCES

Wikipedia

MS (EI): Scopolamine
Lot #89H1298

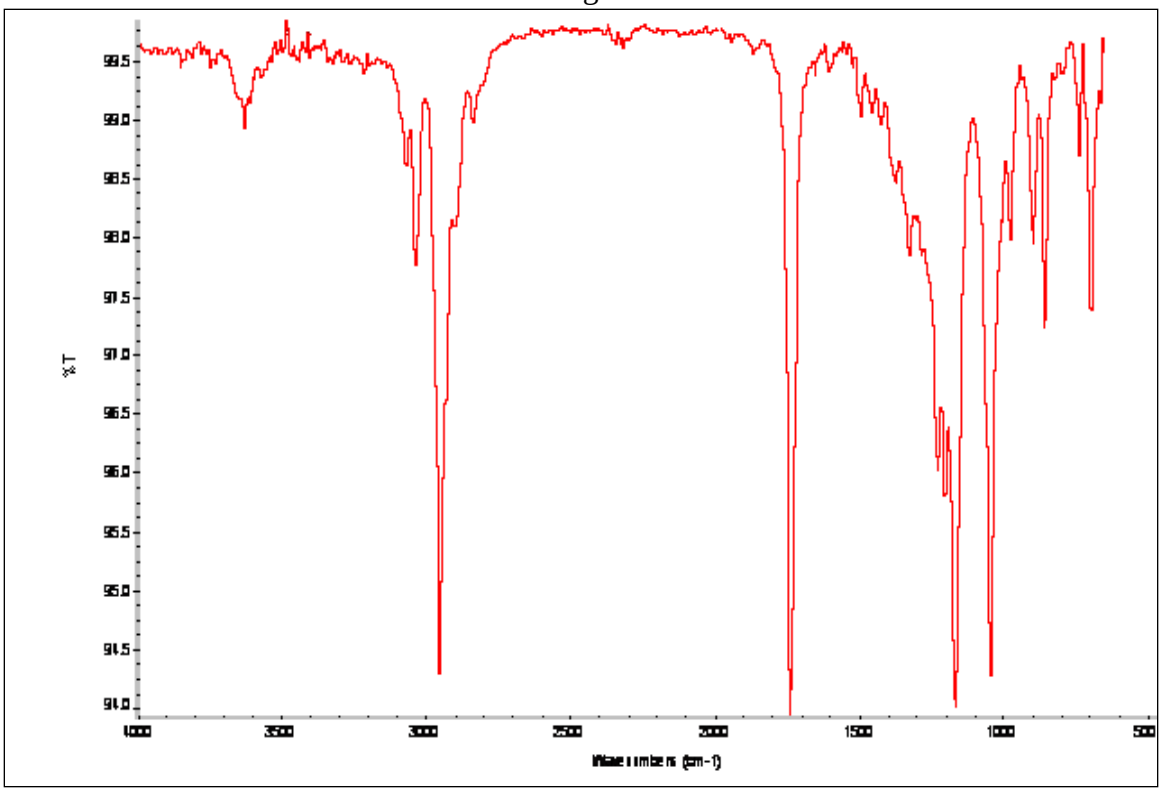


FTIR (One bounce ATR): Scopolamine HBr
Lot #89H1298
4cm^{-1} resolution 32 scans

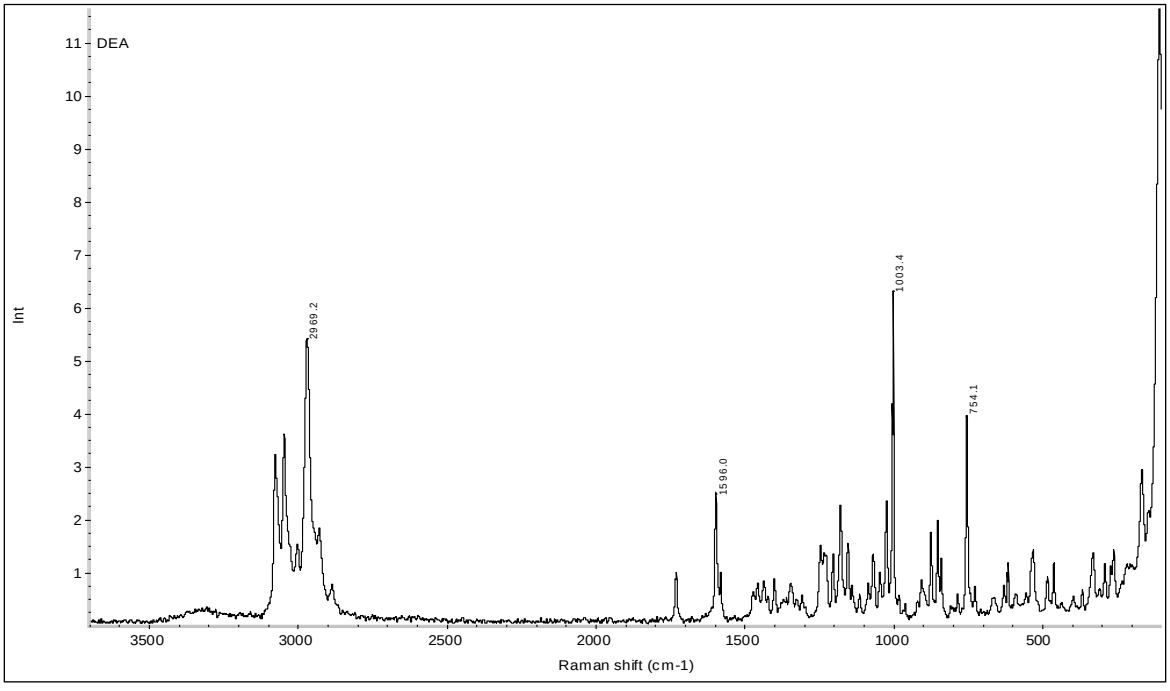


GCIRD: Scopolamine

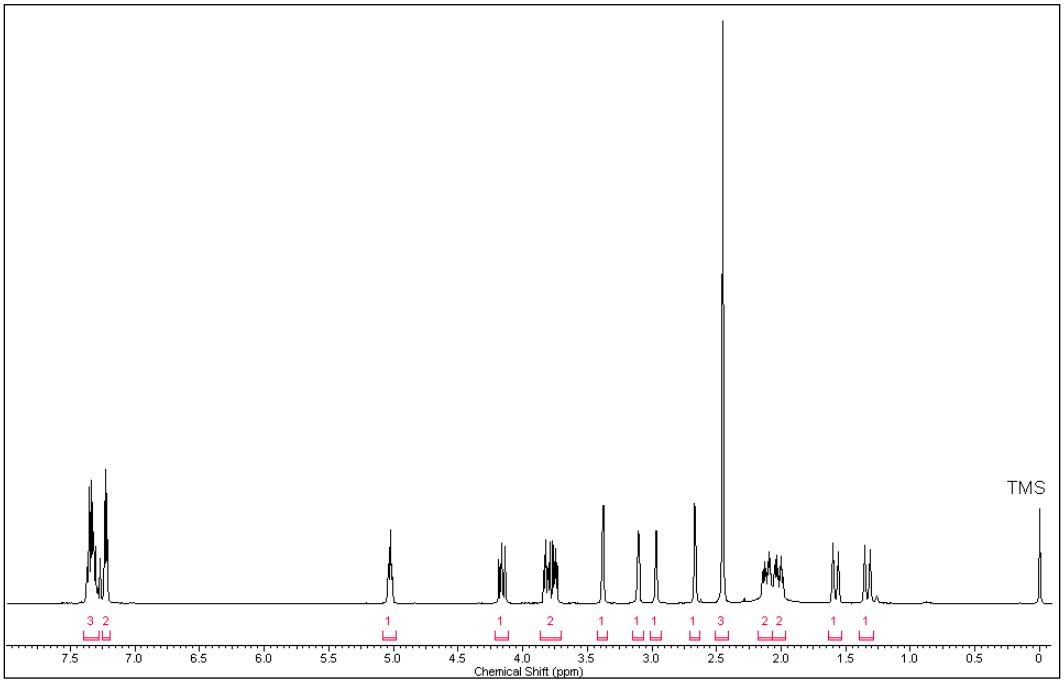
Lot #89H1298
4cm^{-1} resolution 2mg/mL in chloroform



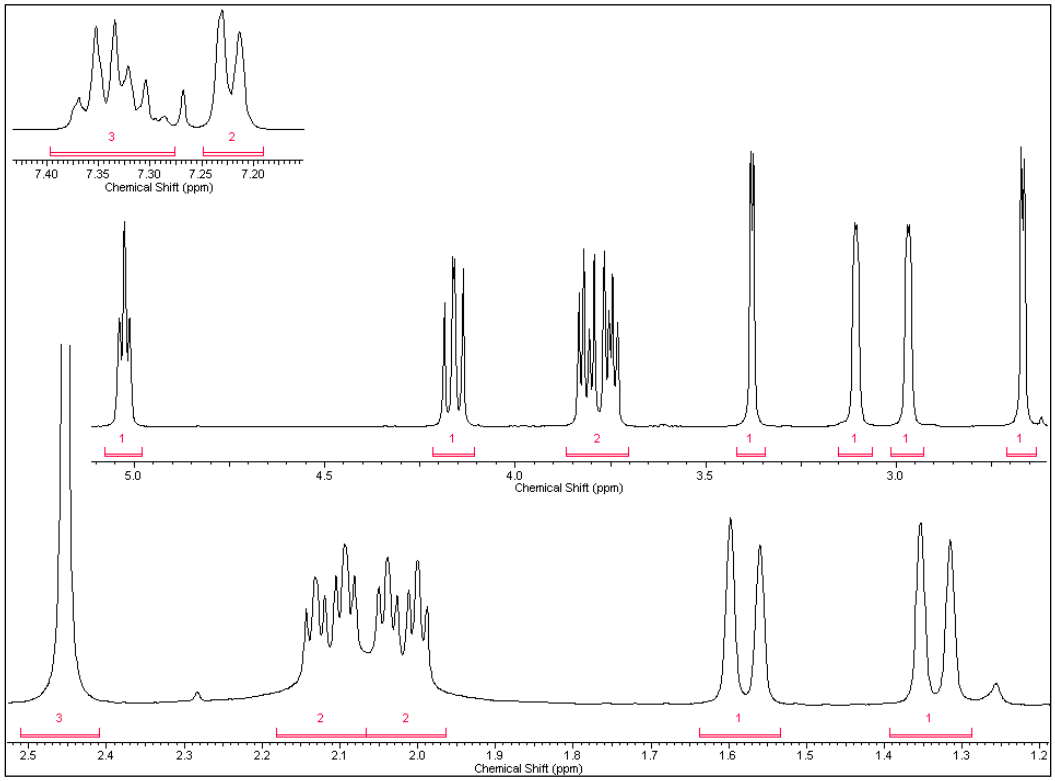
FT-RAMAN: Scopolamine HBr
Lot #89H1298
4cm^{-1} resolution 32 scans



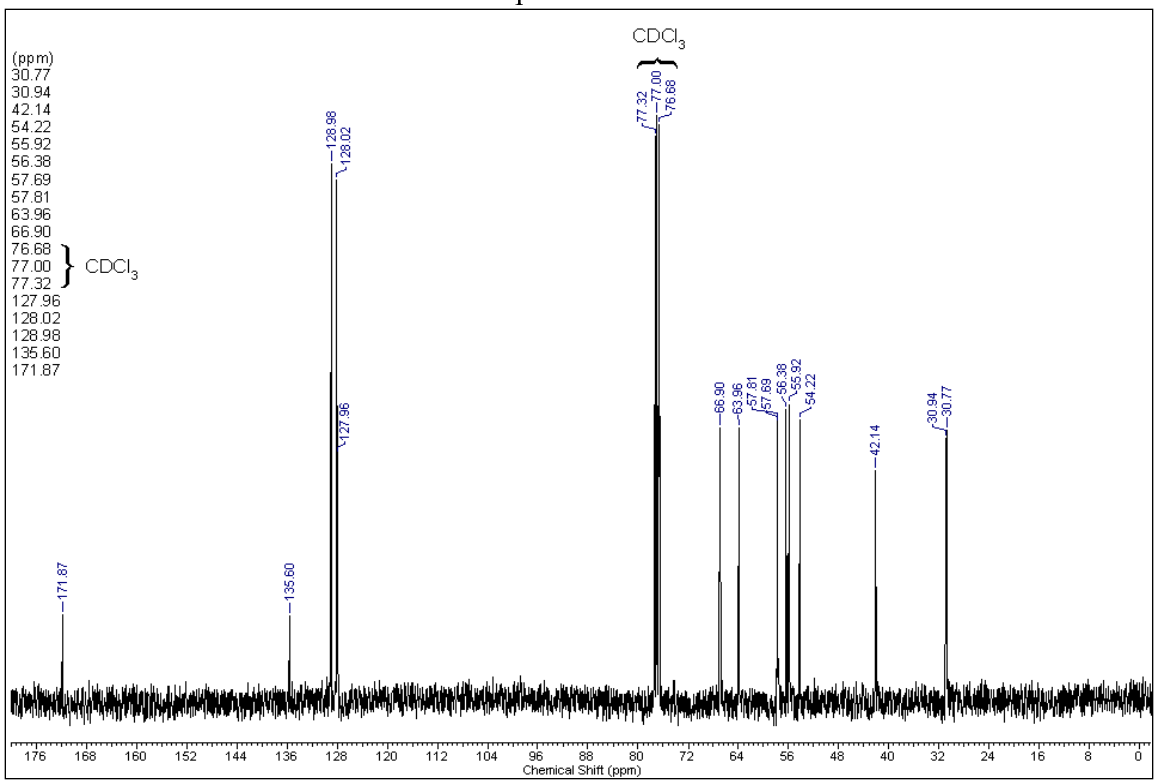
NMR (PROTON): Scopolamine Base chloroform-d with TMS, 400 MHz
Extracted from Scopolamine HBr Lot #89H1298



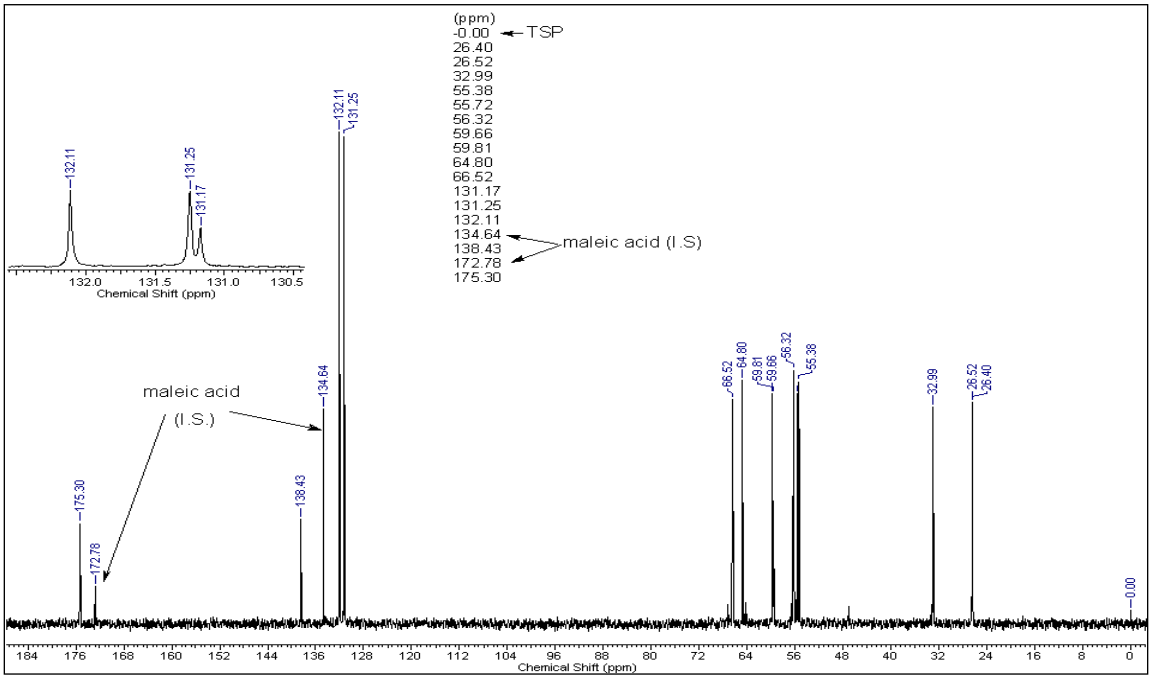
ppm 7.40 - 7.43 (m, 1 H) 7.39 (t, J=1.62 Hz, 1 H) 6.38 (dd, J=1.85, 0.69 Hz, 1 H) 5.53 (dd, J=11.68, 5.20 Hz, 1 H) 5.15 (dd, J=10.52, 9.60 Hz, 1 H) 3.73 (s, 3 H) 2.70 - 2.81 (m, 1 H) 2.51 (dd, J=13.53, 5.20 Hz, 1 H) 2.32 (d, J=9.71 Hz, 1 H) 2.30 (dd, J=13.40, 5.09 Hz, 1 H) 2.17 (s, 3 H) 2.13 - 2.21 (m, 2 H) 2.07 (dd, J=11.91, 3.12 Hz, 1 H) 1.76 - 1.84 (m, 1 H) 1.62 - 1.71 (m, 1 H) 1.52 - 1.62 (m, 2 H) 1.46 (s, 3 H) 1.12 (s, 3 H)



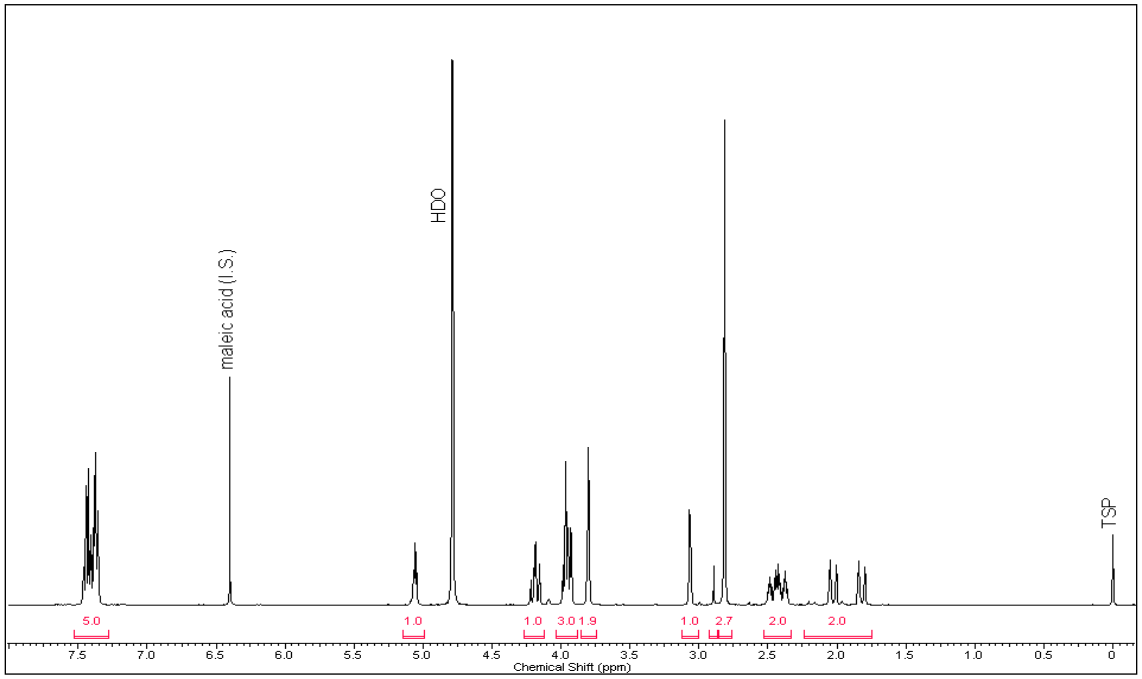
NMR (CARBON): Scopolamine Base, Chloroform-d with TMS
Extracted from Scopolamine HBr Lot #89H1298



NMR (CARBON): Scopolamine HBr
deuterium oxide, maleic acid as internal standard, Lot #89H1298



NMR (PROTON): Scopolamine HBr, 400 MHz
deuterium oxide, maleic acid as internal standard, Lot #89H1298



ppm 7.32 - 7.49 (m, 5 H) 5.06 (t, J=5.0 Hz, 1 H) 4.13 - 4.24 (m, 1 H) 3.90 - 4.00 (m, 3 H) 3.76 - 3.84 (m, 2 H) 3.06 (d, J=3.5 Hz, 1 H) 2.82 (s, 3 H) 2.46 (dt, J=17.3, 4.6 Hz, 1 H) 2.40 (dt, J=17.6, 4.6 Hz, 1 H) 2.03 (d, J=17.2 Hz, 1 H) 1.82 (d, J=17.4 Hz, 1 H)