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PRODUCT NAME Isomitraphylline

PART NUMBER 00009417

STANDARD TYPE Primary (P)

LOT NUMBER 00009417-11B

REPORT NUMBER CDXA-RSS-5860-01

SAMPLE NUMBER CDXA-13-7482

DATE OF SAMPLE 09/30/2013

DATE OF RE-EVALUATION 11/02/2018

DATE OF REPORT 11/30/2018

CHEMICAL NAMES 7-Isomitraphylline; Ajmalicine oxindole A

CHEMICAL FORMULA C₂₁H₂₄N₂O₄

MOLECULAR WEIGHT (MW) 368.43

CHEMICAL FAMILY Alkaloids

CAS NUMBER [4963-01-3]

EC#(EINECS) NA

RTECS WH1312422

Structure HIIIII ΞH

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT
Adjusted Purity	NA	NA	90.0%
HPLC	99.1-04-1.0-000684	NA	97.9%
NMR	99.1-CD-1.0-000122	Conforms to structure	Conforms to structure
Mass Spectrum	Direct Infusion, ESI (-)	Conforms	Conforms
Residual Solvent	99.1-CD-7.0-000115	NA	Dichloromethane – 0.4%; Ethyl acetate – 1.6%; Chloroform – 5.2%
Water	99.1-04-9.0-000094	NA	0.9%
Appearance NA		NA	White powder

ADJUSTED PURITY: 90.0% IS BASED ON (100 - 7.2 SOLVENTS - 0.9 WATER) X 97.9% HPLC

STORAGE CONDITIONS

STORAGE -20 °C in a dry place.

EXPIRATION DATE 11/2023 under the above conditions.







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ANALYTICAL CONDITIONS

INSTRUMENT AGILENT 1260 HPLC UV-VIS (DAD)

AGILENT 6510 QTOF

COLUMN Phenomenex Luna C18(2) 150 x 2.00 mm, 5 µm particle size

MOBILE PHASE A - 0.1% Trifluoroacetic acid in Ultrapure water, B - Acetonitrile;

Isocratic 5% B for 5 minutes, then increasing to 95% B over 20 minutes. Hold at

95% B for 15 minutes.

60 °C COLUMN TEMP.

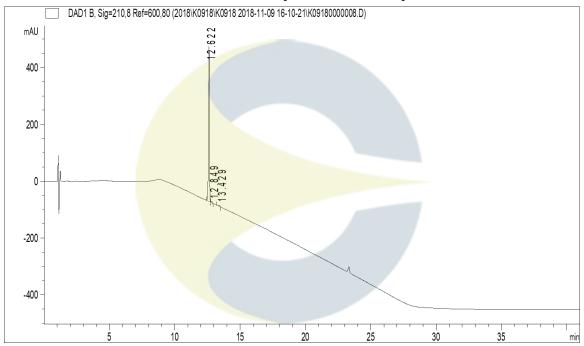
FLOW RATE 0.4 mL/minute

INJECTION VOL. $0.4 \mu L$

INJECTION CONC. 0.7 mg/mL in Methanol

DETECTION $210 \pm 4 \text{ nm}$

HPLC CHROMATOGRAM OF ISOMITRAPHYLLINE (CDXA-13-7482)



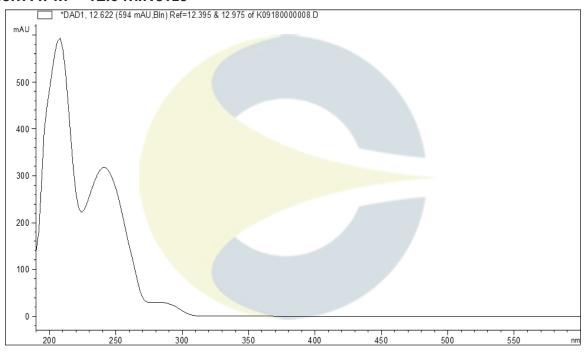




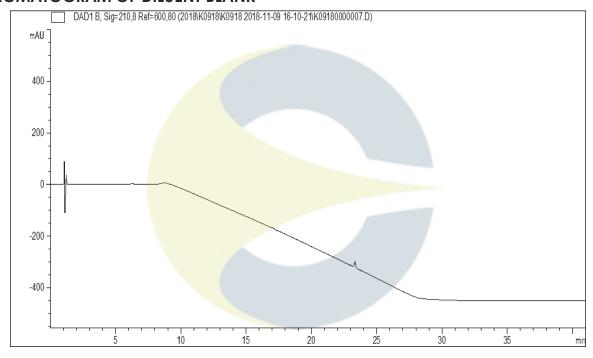


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UV SPECTRUM AT RT = 12.6 MINUTES



HPLC CHROMATOGRAM OF DILUENT BLANK



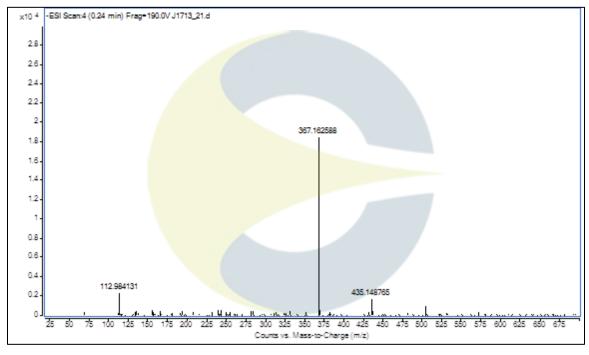




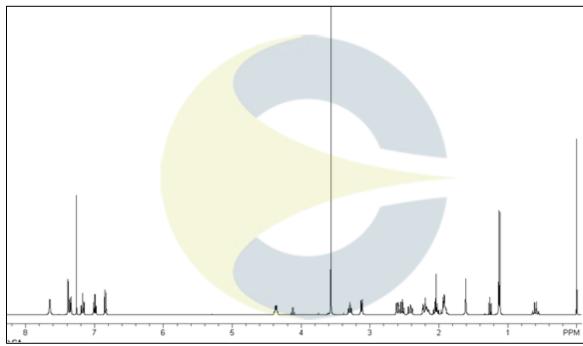


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MASS SPECTRUM OF ISOMITRAPHYLLINE (CDXA-13-7482)



¹H-NMR SPECTRUM OF ISOMITRAPHYLLINE (CDXA-13-7482) IN CDCI₃



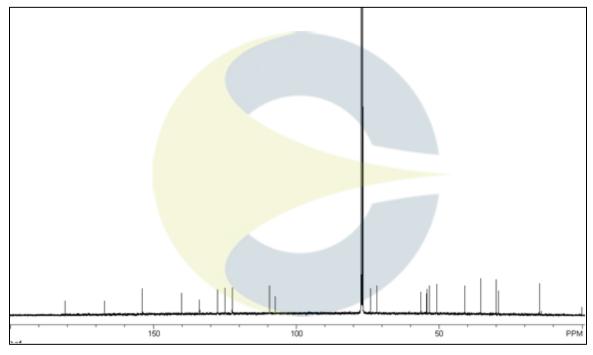






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¹³C-NMR SPECTRUM OF ISOMITRAPHYLLINE (CDXA-13-7482) IN CDCI₃



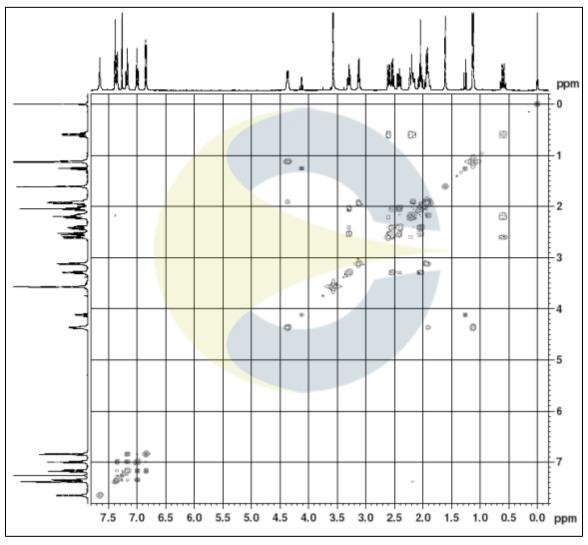






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COSY-NMR SPECTRUM OF ISOMITRAPHYLLINE (CDXA-13-7482) IN CDCI₃



REVISION HISTORY

Revision History	<u>Date of Revision</u>	Document/Changes
00	10/23/2013	New report
01	11/30/2018	Passed re-evaluation by HPLC and water content. Updated Results, Analytical Conditions, chromatograms, UV spectrum, structure and expiration date. Added RTECS

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