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PRODUCT NAME Methysticin

PART NUMBER 00013860

STANDARD TYPE Primary (P)

LOT NUMBER 00013860-711

REPORT NUMBER CDXA-RSS-4604-02

SAMPLE NUMBER CDXA-11-4302

DATE OF SAMPLE 07/26/2011

DATE OF RE-EVALUATION 10/15/2015 (1st); 09/01/2020 (2nd)

DATE OF REPORT 09/14/2020

(6R)-6-[(1E)-2-(1,3-Benzodioxol-5-yl)ethenyl]-5,6-dihydro-4-methoxy-2H-pyran-2-

one; (+)-Methysticin; Kavatin **CHEMICAL NAMES**

CHEMICAL FORMULA C₁₅H₁₄O₅

274.27 MOLECULAR WEIGHT (MW)

CHEMICAL FAMILY Kavalactones

CAS NUMBER [495-85-2]

EC#(EINECS) NA

RTECS UQ0517000

Structure

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT	
Adjusted Purity	NA	NA	99.7%	
HPLC	0.700.10.2.METH22	NA	99.7%	
NMR	99.1-CD-1.0-000122	Conforms to structure	Conforms to structure Conforms ND	
Mass Spectrum	Direct Infusion, ESI (+)	Conforms		
Residual Solvent*	99.1-CD-4.0-000115	NA		
Water 0.700.12.37 Appearance NA		NA	ND	
		NA	NA White powder	

99.7% IS BASED ON (100 - 0.0 SOLVENTS - 0.0 WATER) X 99.7% HPLC ADJUSTED PURITY:

STORAGE CONDITIONS

STORAGE -20°C in a dry place.

EXPIRATION DATE 09/2025 under the above conditions.

Digitally signed by Elizabeth Hughes Quality Assurance Elizabeth Hughes **Specialist** Assistant Date: 2020.09.14 Designee of QA Management 10:13:42 -06'00'







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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.

COLUMN TEMP. 60 °C

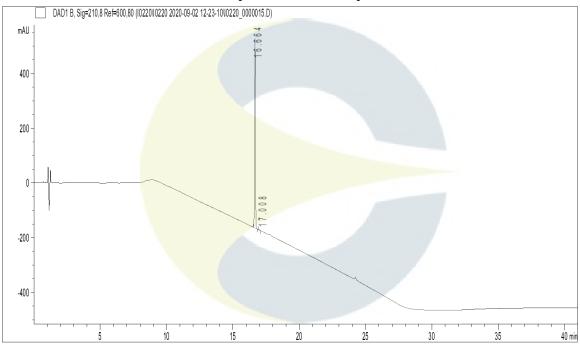
FLOW RATE 0.4 mL/minute

INJECTION VOL. 0.2 μL

INJECTION CONC. 1.0 mg/mL in Methanol

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

HPLC CHROMATOGRAM OF METHYSTICIN (CDXA-11-4302)



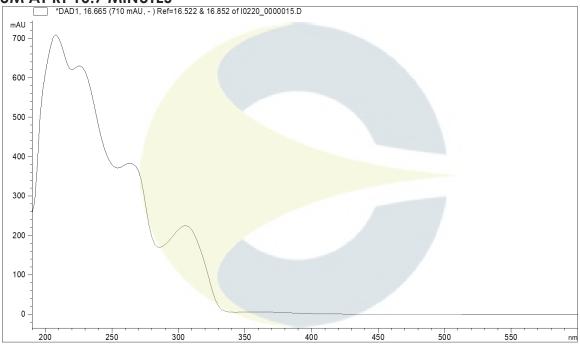




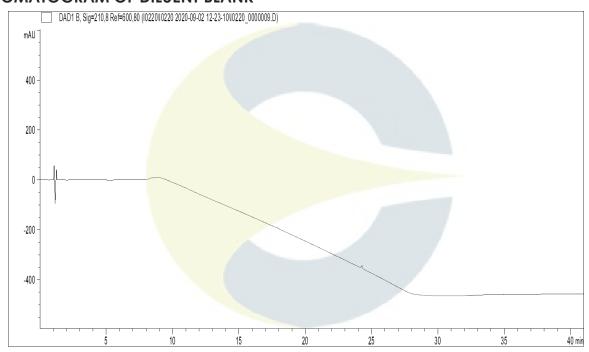


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UV SPECTRUM AT RT 16.7 MINUTES



HPLC CHROMATOGRAM OF DILUENT BLANK



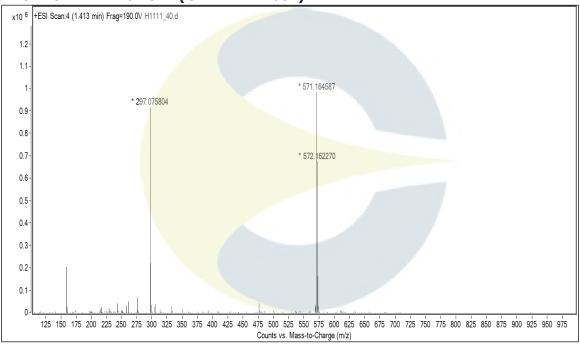




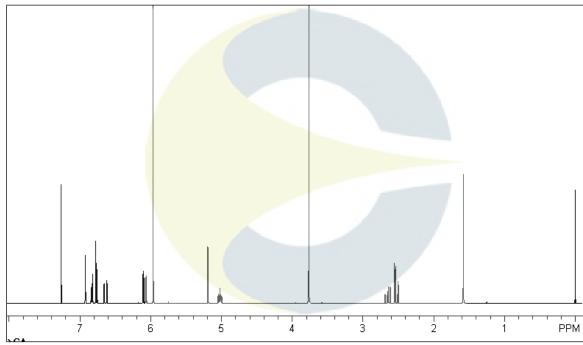


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MASS SPECTRUM OF METHYSTICIN (CDXA-11-4302)



¹H-NMR SPECTRUM OF METHYSTICIN (CDXA-11-4302) IN CDCI₃



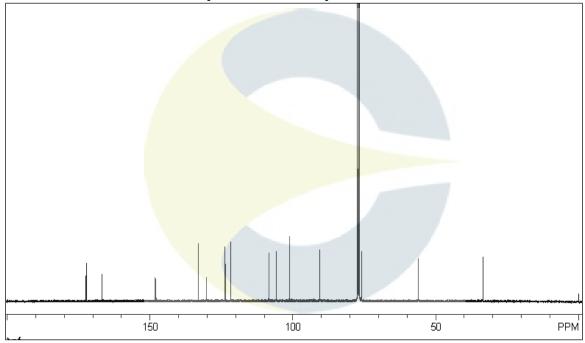






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13C-NMR SPECTRUM OF METHYSTICIN (CDXA-11-4302) IN CDCI₃



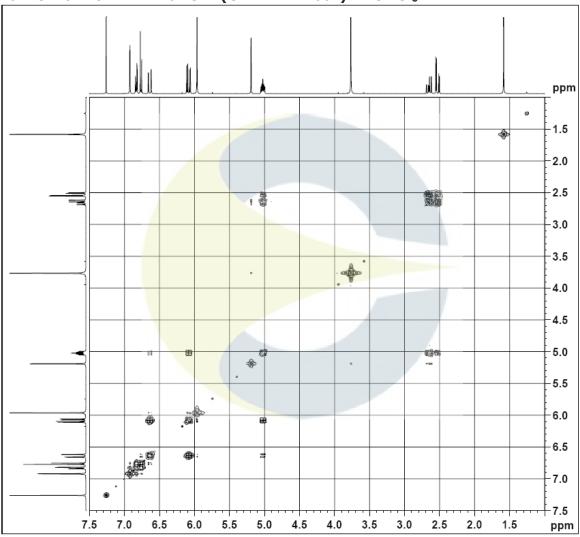






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COSY-NMR SPECTRUM OF METHYSTICIN (CDXA-11-4302) IN CDCI₃



REVISION HISTORY

<u>Revision History</u>	<u>Date of Revision</u>	<u>Document/Changes</u>
00	08/24/2011	New report
01	11/05/2015	Passed re-evaluation by HPLC. Updated expiration date.
02	09/14/2020	Passed second re-evaluation by HPLC and KF. Updated analytical results, expiration date, analytical conditions, chromatograms, UV spectrum, and removed melting point.