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Structure

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PRODUCT NAME Isosteviol

PART NUMBER 00009591

STANDARD TYPE Primary (P)

LOT NUMBER 00009591-802

REPORT NUMBER CDXA-RSS-8019-02

SAMPLE NUMBER CDXP-18-00413

DATE OF SAMPLE 05/02/2018

DATE OF RE-EVALUATION 07/12/2022

DATE OF REPORT 08/03/2022

CHEMICAL NAMES $(4\alpha,8\beta,13\beta)$ -13-Methyl-16-oxo-17-norkauran-18-oic acid; Ketoisostevic acid

CHEMICAL FORMULA C₂₀H₃₀O₃

MOLECULAR WEIGHT (MW) 318.45

CHEMICAL FAMILY Diterpenes

CAS NUMBER [27975-19-5]

EC#(EINECS) 817-156-8

RTECS RC5532500

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT	
Adjusted Purity	NA	≥ 85%	99.5%	
HPLC	0.700.10.2.METH86	≥ 90%	99.8% Conforms to structure	
NMR	99.1-04-2.0-000122	Conforms to structure		
Mass Spectrum	99.1-04-3.0-000126	Conforms	Conforms	
Residual Solvent*	99.1-CDXA-3.0-000621	NA	EtOAc - 0.3%	
Water	0.700.12.37	NA	ND	
Appearance	Appearance NA		White powder	

*Testing performed at an ISO 17025 accredited subcontracted laboratory.

99.5% IS BASED ON (100 - 0.3 SOLVENTS - 0.0 WATER) X 99.8% HPLC ADJUSTED PURITY:

STORAGE CONDITIONS

STORAGE Room Temperature in a dry place. **EXPIRATION DATE** 07/2027 under the above conditions.







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ANALYTICAL CONDITIONS

INSTRUMENT AGILENT 1260 HPLC UV-VIS (DAD); AB-SCIEX 6600 TRIPLE TOF

COLUMN Phenomenex Synergi Hydro RP 80A 250 x 4.6 mm, 4 µm particle size

MOBILE PHASE A – Ultrapure water, B - Acetonitrile;

Isocratic 20% B for 5 minutes, then increasing to 30% B over 10 minutes, then increasing to 35% B over 15 minutes, then increasing to 80% over 10 minutes, then increasing to 80% over 10 minutes,

then increasing to 90% over 5 minutes, hold at 90% for 5 minutes, then

decreasing to 20% over 1 minute.

COLUMN TEMP. 60 °C

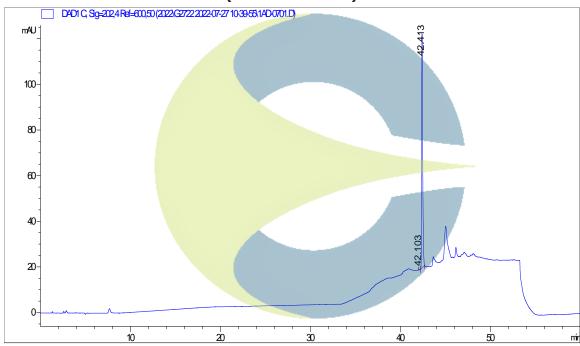
FLOW RATE 1.0 mL/minute

INJECTION VOL. 10 μL

INJECTION CONC. 1.0 mg/mL in (8:2) Acetonitrile: Ultrapure Water

DETECTION $202 \pm 2 \text{ nm}$

HPLC CHROMATOGRAM OF ISOSTEVIOL (CDXP-18-00413)





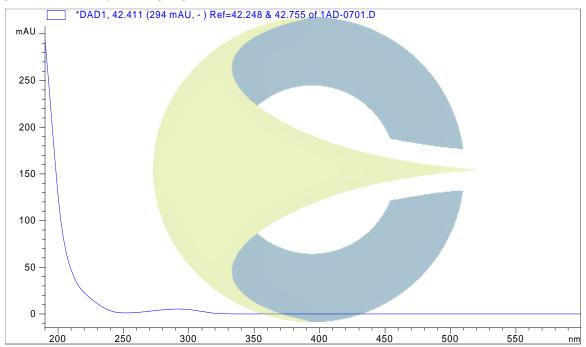




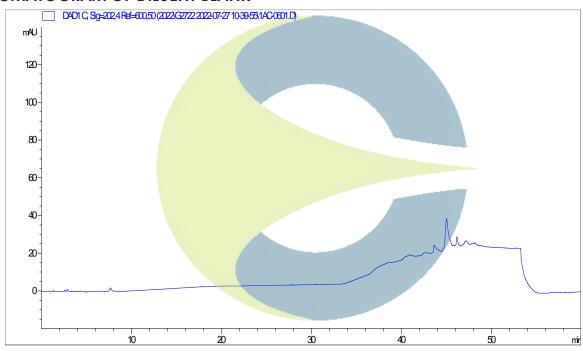
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UV SPECTRUM AT RT = 42.4 MINUTES



HPLC CHROMATOGRAM OF DILUENT BLANK





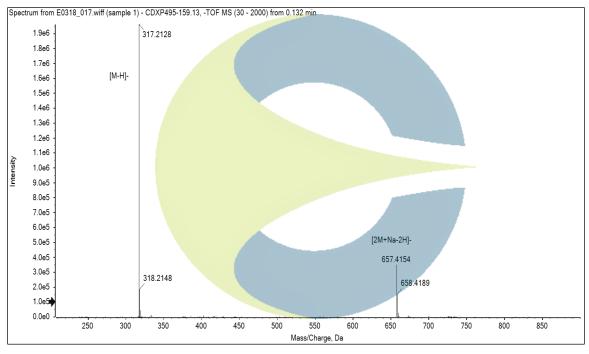




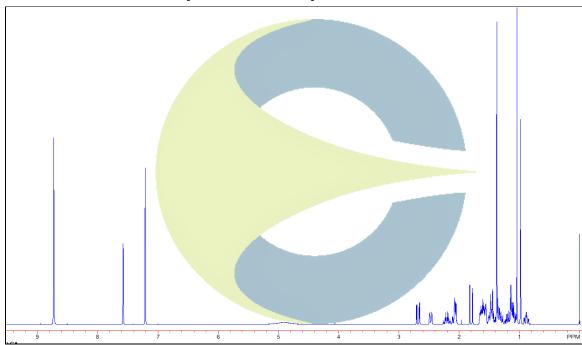
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MASS SPECTRUM OF ISOSTEVIOL (CDXP-18-00413)



¹H-NMR SPECTRUM OF ISOSTEVIOL (CDXP-18-00413) IN PYRIDINE-d₅





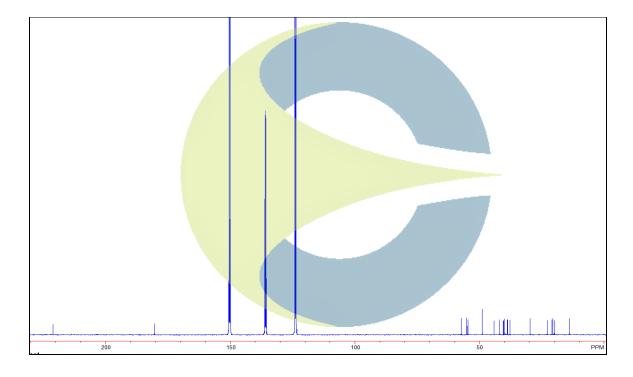




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¹³C-NMR SPECTRUM OF ISOSTEVIOL (CDXP-18-00413) IN PYRIDINE-d₅





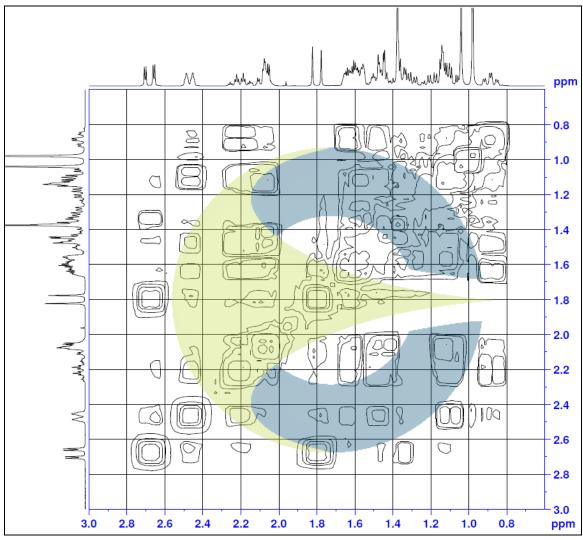




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COSY-NMR SPECTRUM OF ISOSTEVIOL (CDXP-18-00413) IN PYRIDINE-d5



REVISION HISTORY

<u>Revision History</u>	<u>Date of Revision</u>	<u>Document/Changes</u>
00	05/29/2018	New report
01	08/31/2018	Corrected water content result.
02	08/03/2022	Passed re-evaluation by HPLC, KF. Updated expiration date, analytical method, conditions, chromatograms and results. Added EINECS number.