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PRODUCT NAME Linustatin

PART NUMBER 00012282

STANDARD TYPE Primary (P)

LOT NUMBER 00012282-3243

REPORT NUMBER CDXA-RSS-4544-02

SAMPLE NUMBER CDXA-11-3243

DATE OF SAMPLE 05/20/2011

DATE OF RE-EVALUATION 06/08/2015 (1st); 07/22/2019 (2nd)

DATE OF REPORT 08/20/2019 Structure

CHEMICAL NAMES 2-[(6-O-β-D-Glucopyranosyl-β-D-glucopyranosyl)oxy]-2-methylpropanenitrile

CHEMICAL FORMULA C₁₆H₂₇NO₁₁

MOLECULAR WEIGHT (MW) 409.39

CHEMICAL FAMILY Cyanogenic Glucosides

CAS NUMBER [72229-40-4]

EC#(EINECS) NA

RTECS TZ4805000

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT	
Adjusted Purity	NA	NA	87.1%	
HPLC	CDXA-CPM-100-00	NA	95.9%	
NMR	99.1-CD-1.0-000122	Conforms to structure	Conforms to structure Conforms Acetone – 1.2%	
Mass Spectrum	Direct Infusion, ESI (–)	Conforms		
Residual Solvent	99.1-CD-4.0-000115	NA		
Water	Water 0.700.12.37		8.0%	
Appearance	NA	NA	White powder	

ADJUSTED PURITY: 87.1% IS BASED ON (100 - 1.2 SOLVENTS - 8.0 WATER) X 95.9% HPLC

STORAGE CONDITIONS

STORAGE +4 °C in a dry place.

EXPIRATION DATE 07/2024 under the above conditions.







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ANALYTICAL CONDITIONS

INSTRUMENT AGILENT 1260 HPLC UV-VIS (DAD) CONNECTED TO DIONEX CORONA VEO

CHARGED AEROSOL DETECTOR (CAD); AGILENT 6510 QTOF

COLUMN Shodex Asahipak NH2-40 4E, 250 x 4.60 mm, 5 µm particle size

MOBILE PHASE A – Ultrapure Water;

Isocratic 100% A for 31 minutes.

60 °C COLUMN TEMP.

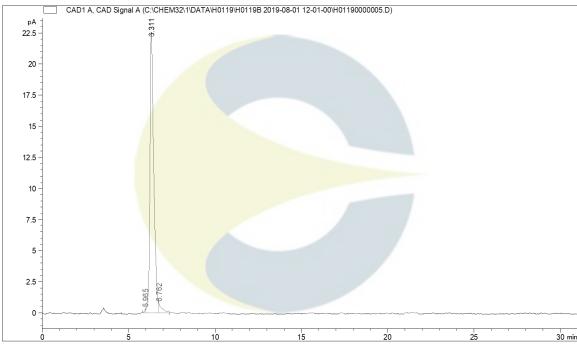
FLOW RATE 0.4 mL/minute

INJECTION VOL. 5.0 µL

INJECTION CONC. 2.1 mg/mL in Ultrapure Water

DETECTION CAD

HPLC CHROMATOGRAM OF LINUSTATIN (CDXA-11-3243)



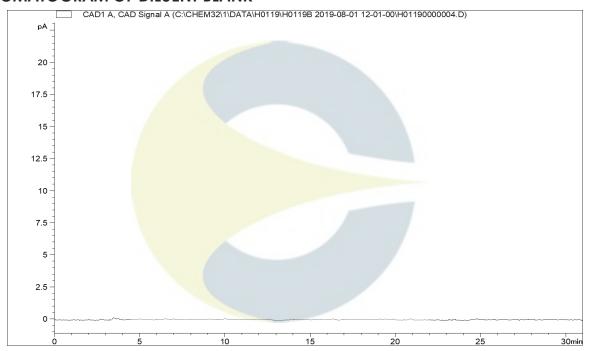




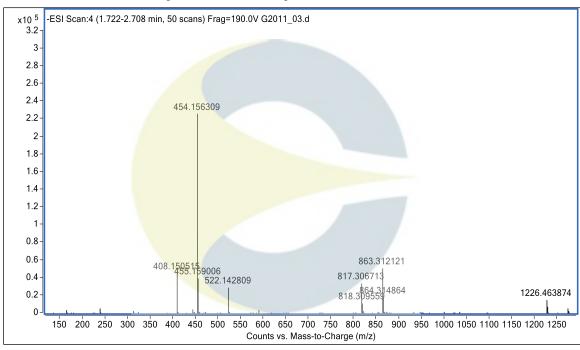


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HPLC CHROMATOGRAM OF DILUENT BLANK



MASS SPECTRUM OF LINUSTATIN (CDXA-11-3243)



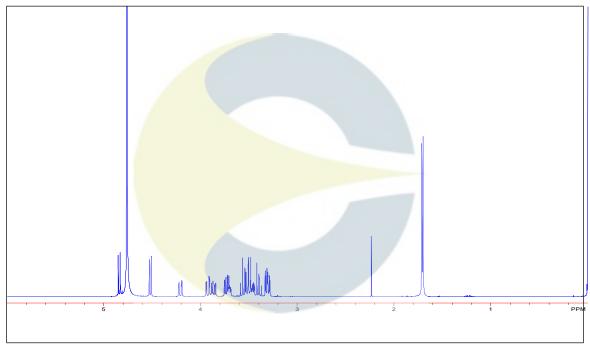




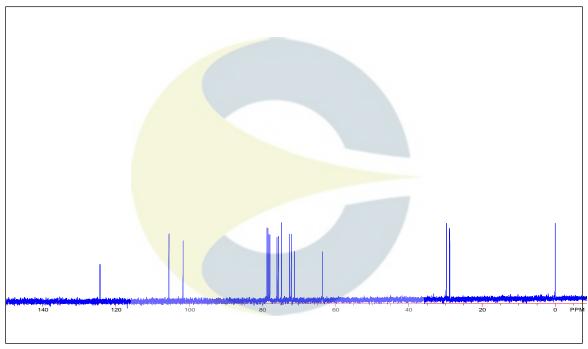


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¹H-NMR SPECTRUM OF LINUSTATIN (CDXA-11-3243) IN D₂O



13C-NMR SPECTRUM OF LINUSTATIN (CDXA-11-3243) IN D2O









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REVISION HISTORY

Revision History	<u>Date of Revision</u>	<u>Document/Changes</u>
00	7/21/2011	New report
01	06/30/2015	Passed re-evaluation by HPLC and KF. Updated expiration date, updated melting point, and updated template.
02	08/20/2019	Passed second re-evaluation by HPLC, KF. Updated expiration date, analytical method, conditions, chromatograms and results. Removed melting point and added RTECS number.