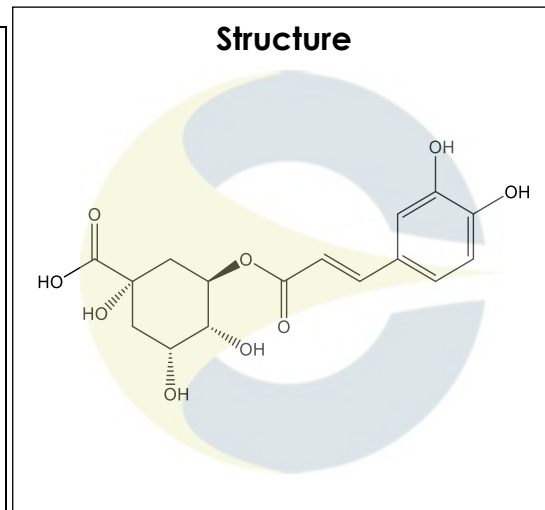


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PRODUCT NAME	Chlorogenic acid
PART NUMBER	00003450
STANDARD TYPE	Primary (P)
LOT NUMBER	00003450-550
REPORT NUMBER	CDXA-RSS-8457-01
SAMPLE NUMBER	CDXP-18-01362
DATE OF SAMPLE	01/02/2019
DATE OF RE-EVALUATION	12/09/2021
DATE OF REPORT	12/20/2021



CHEMICAL NAMES	(1S,3R,4R,5R)-3-[[3-(3,4-Dihydroxyphenyl)-1-oxo-2-propen-1-yl]oxy]-1,4,5-trihydroxy-cyclohexanecarboxylic acid; 3-Caffeoylquinic acid
CHEMICAL FORMULA	C ₁₆ H ₁₈ O ₉
MOLECULAR WEIGHT (MW)	354.31
CHEMICAL FAMILY	Phenolic acids
CAS NUMBER	[327-97-9]
EC#(EINECS)	206-325-6
RTECS	GU8480000

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT
Adjusted Purity	NA	≥ 85%	97.2%
HPLC	0.700.10.2.METH22	≥ 90%	99.6%
NMR	30.1-04-1.0-000733	Conforms to structure	Conforms to structure
Mass Spectrum	99.1-04-3.0-000126	Conforms	Conforms
Residual Solvent	99.1-CDXA-3.0-000621	NA	ND
Water	0.700.12.37	NA	2.4%
Appearance	NA	NA	White powder

ADJUSTED PURITY: 97.2% IS BASED ON (100 - 0.0 SOLVENTS - 2.4 WATER) X 99.6% HPLC

STORAGE CONDITIONS

STORAGE	Room Temperature in a dry place.
EXPIRATION DATE	12/2026 under the above conditions.

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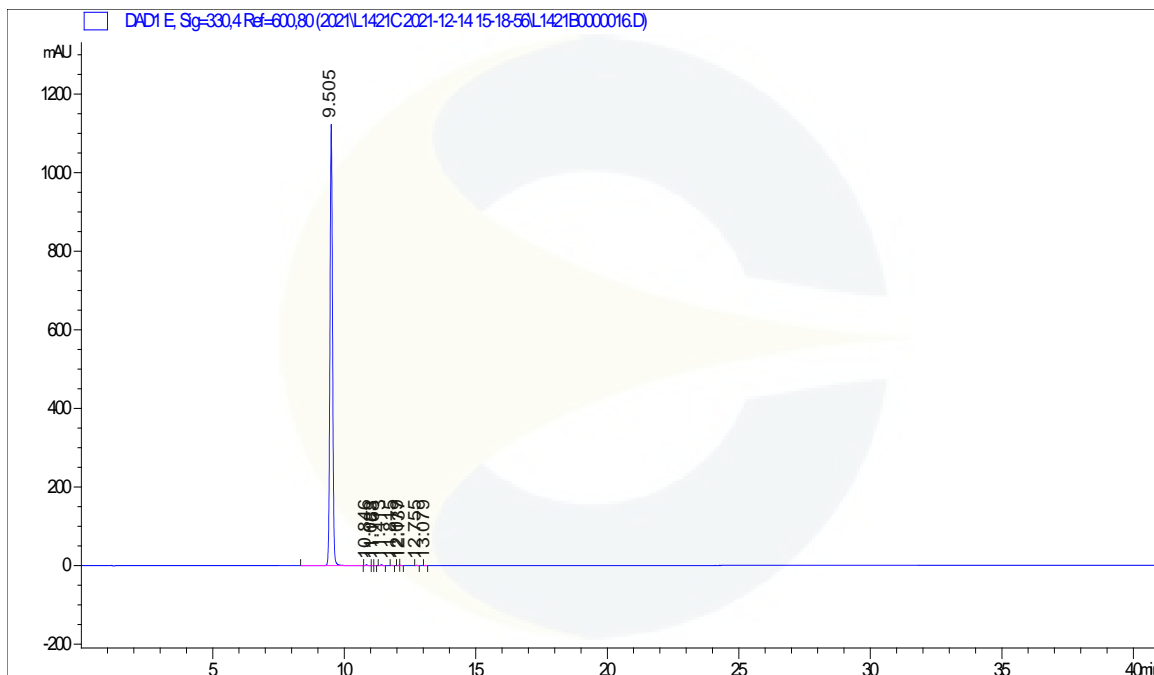
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ANALYTICAL CONDITIONS

INSTRUMENT	AGILENT 1260 HPLC UV-VIS (DAD); AB-SCIEX 6600 TRIPLE TOF
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.	1.0 µL
INJECTION CONC.	1.0 mg/mL in Ethanol
DETECTION	330 ± 2 nm

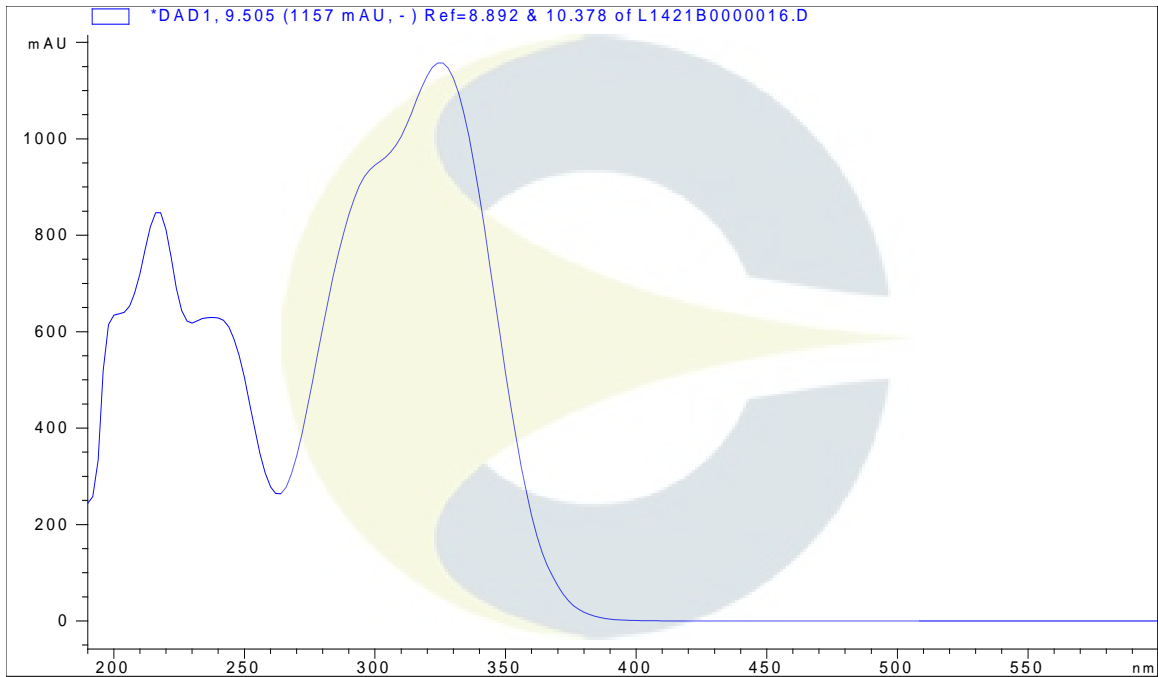
HPLC CHROMATOGRAM OF CHLOROGENIC ACID (CDXP-18-01362)



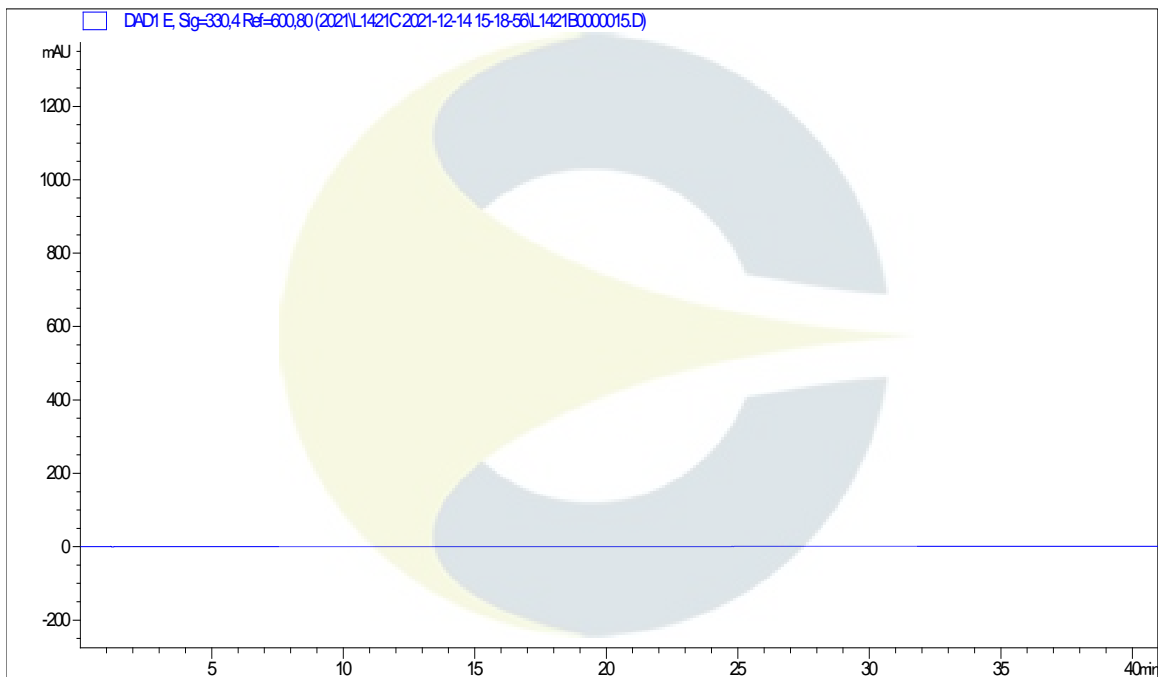
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UV SPECTRUM AT RT = 9.5 MINUTES



HPLC CHROMATOGRAM OF DILUENT BLANK

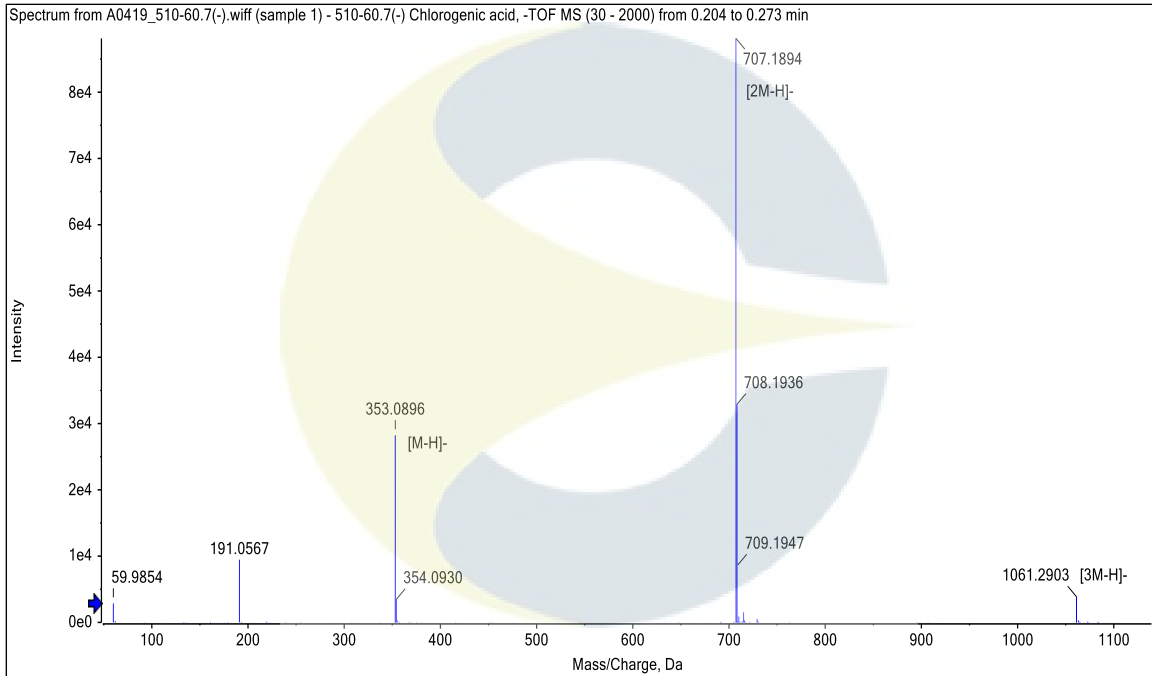


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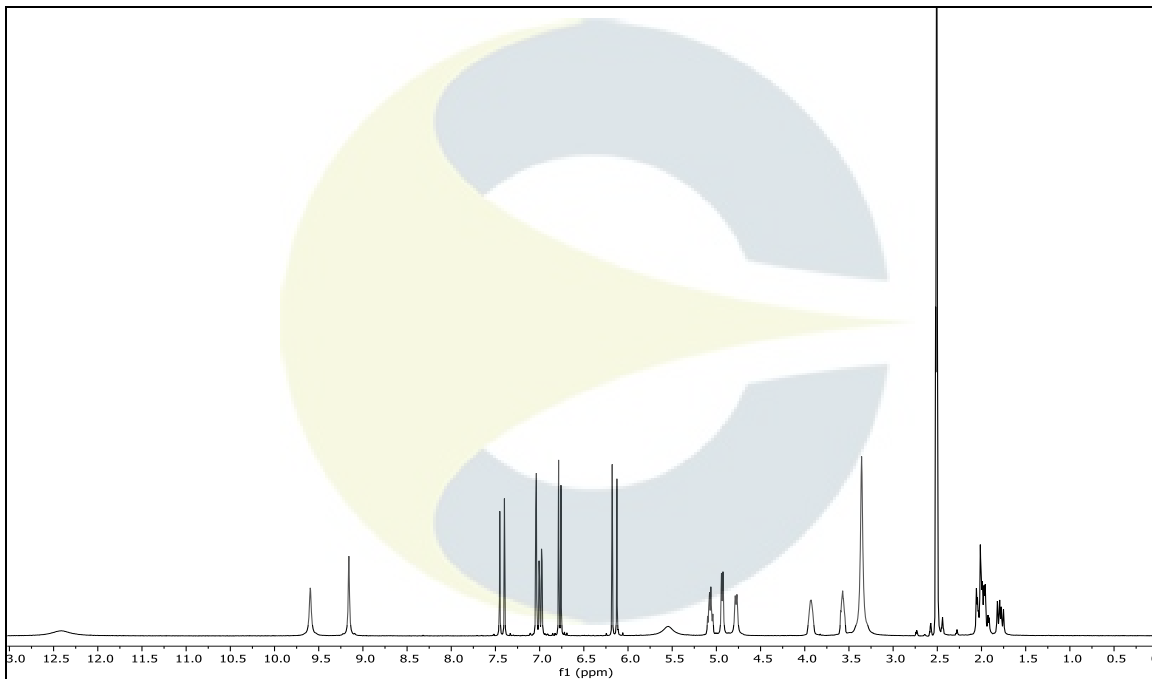
10900 Wilshire Blvd., Suite 600, Los Angeles, CA 90024 | T: +1 949-419-0288 | F: +1 949-419-0294 | www.chromadex.com
 Laboratory address: 1751 S. Fordham St., Suite 350, Longmont, CO 80503

India Contact:
 Life Technologies (India) Pvt. Ltd.
 306, Aggarwal City Mall, Opposite M2K Pitampura, Delhi – 110034 (INDIA). Ph: +91-11-42208000, 42208111, 42208222, Mobile: +91-9810521400, Fax: +91-11-42208444
 Email: customerservice@lifetechindia.com Website: www.lifetechindia.com

MASS SPECTRUM OF CHLOROGENIC ACID (CDXP-18-01362)



¹H-NMR SPECTRUM OF CHLOROGENIC ACID (CDXP-18-01362) IN DMSO-*d*₆

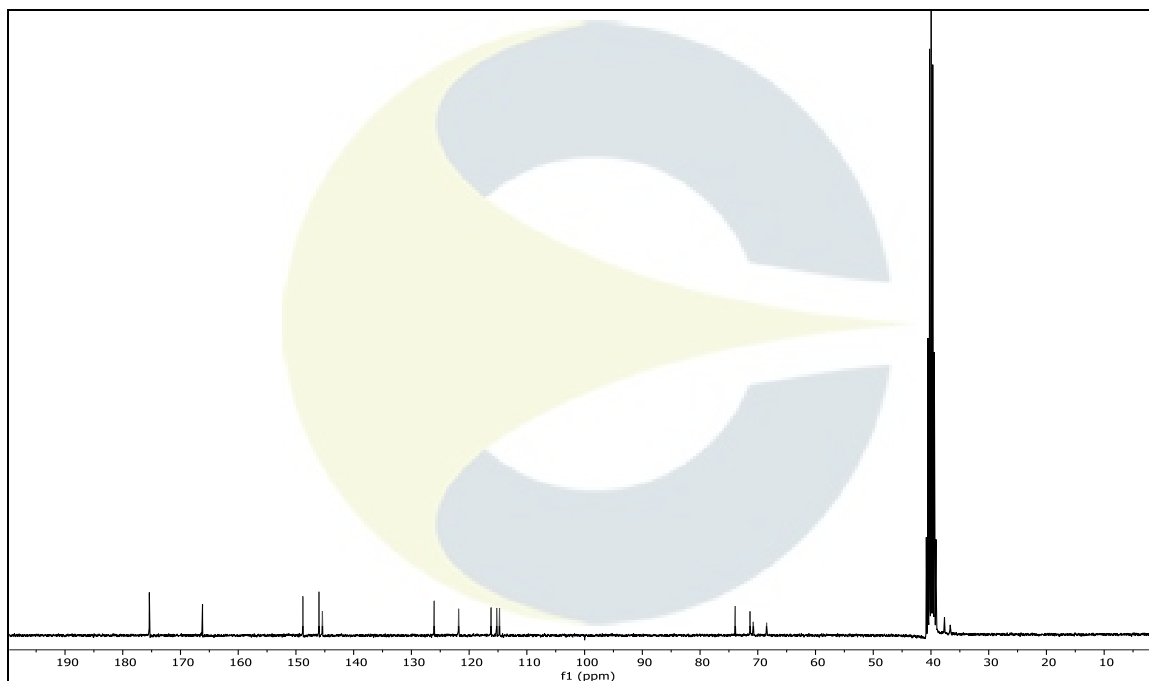


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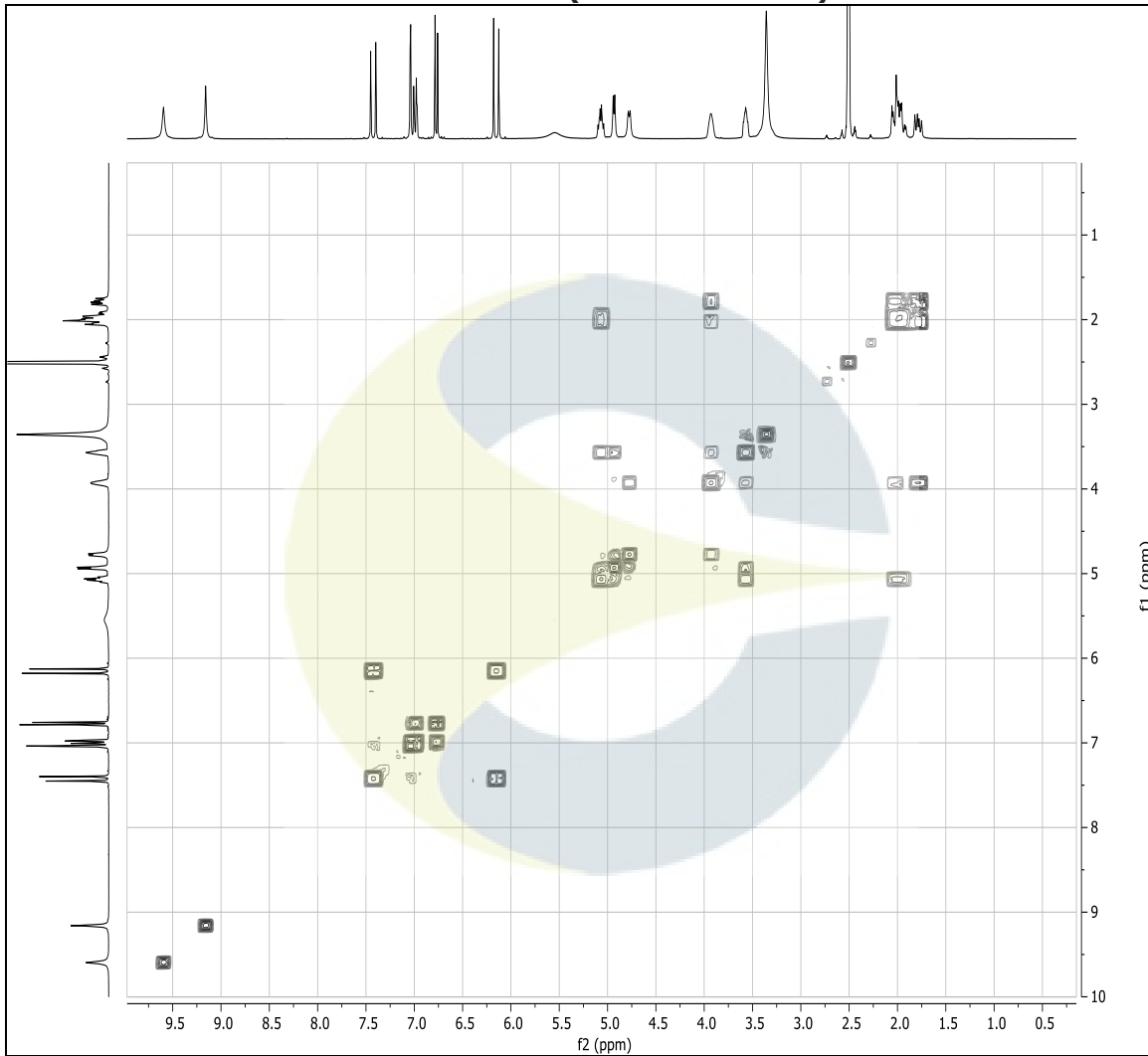
¹³C-NMR SPECTRUM OF CHLOROGENIC ACID (CDXP-18-01362) IN DMSO- d₆



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Email: customerservice@lifetechindia.com Website: www.lifetechindia.com

COSY-NMR SPECTRUM OF CHLOROGENIC ACID (CDXP-18-01362) IN DMSO- *d*₆

REVISION HISTORY

<u>Revision History</u>	<u>Date of Revision</u>	<u>Document/Changes</u>
00	01/28/2019	New report
01	12/20/2021	Passed re-evaluation by HPLC and KF. Updated analytical conditions, results, HPLC chromatograms, and expiration date.

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