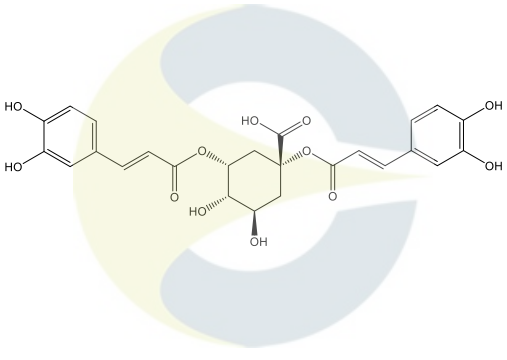


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PRODUCT NAME	1,3-Dicaffeoylquinic acid	<div style="text-align: center;"> Structure  </div>
PART NUMBER	00003991	
STANDARD TYPE	Primary (P)	
LOT NUMBER	00003991-915	
REPORT NUMBER	CDXA-RSS-7269-04	
SAMPLE NUMBER	CDXP-17-00265	
DATE OF SAMPLE	08/29/2016	
DATE OF RE-EVALUATION	09/28/2020	
DATE OF REPORT	02/05/2021	

CHEMICAL NAMES	(1R,3R,4S,5R)-1,3-Bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propen-1-yl]oxy]-4,5-dihydroxy-cyclohexanecarboxylic acid;
CHEMICAL FORMULA	C ₂₅ H ₂₄ O ₁₂
MOLECULAR WEIGHT (MW)	516.45
CHEMICAL FAMILY	Phenolic acids
CAS NUMBER	[30964-13-7]
EC#(EINECS)	N/A
RTECS	N/A

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT
Adjusted Purity	NA	≥ 85%	94.8%
HPLC	0.700.10.2.METH22	≥ 90%	98.7%
NMR	4.5.3-CD-4.0-000338	Conforms to structure	Conforms to structure
Mass Spectrum	99.1CDXA-2.0-000126	Conforms	Conforms
Residual Solvent	99.1-CD-9.0-000115	NA	ND
Water	0.700.12.37	NA	4.0%
Appearance	NA	NA	White powder

ADJUSTED PURITY: 94.8% IS BASED ON (100 - 0.0 SOLVENTS - 4.0 WATER) X 98.7% HPLC

STORAGE CONDITIONS

STORAGE	+4 °C in a dry place.
EXPIRATION DATE	09/2025 under the above conditions.

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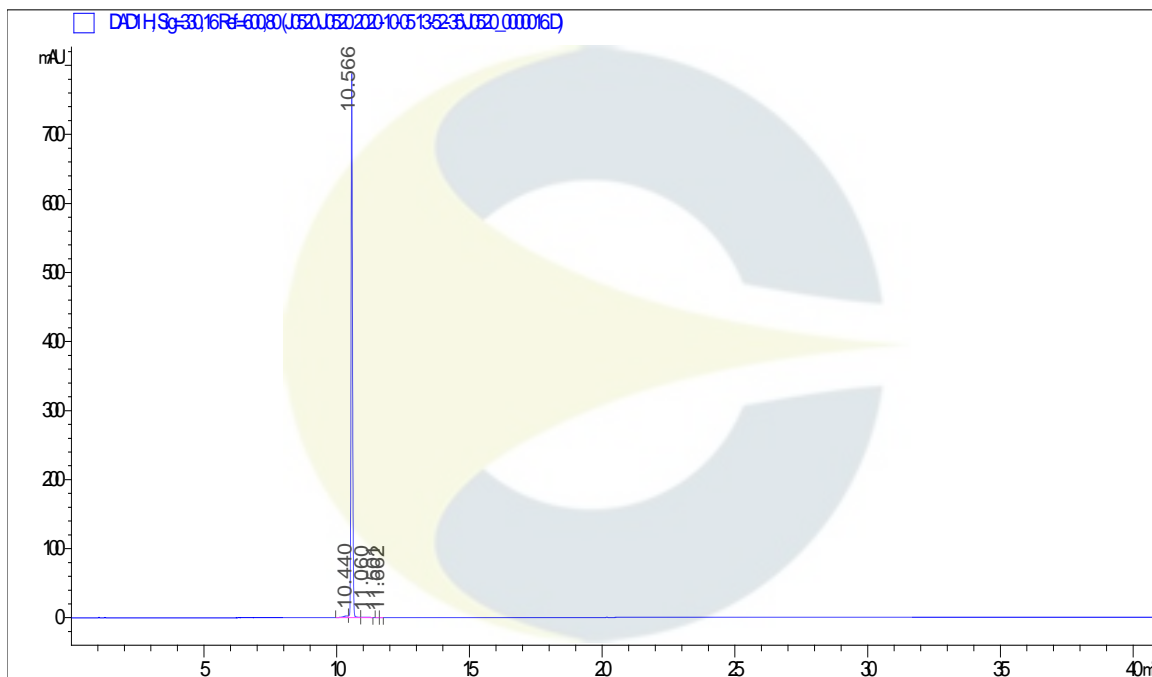
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ANALYTICAL CONDITIONS

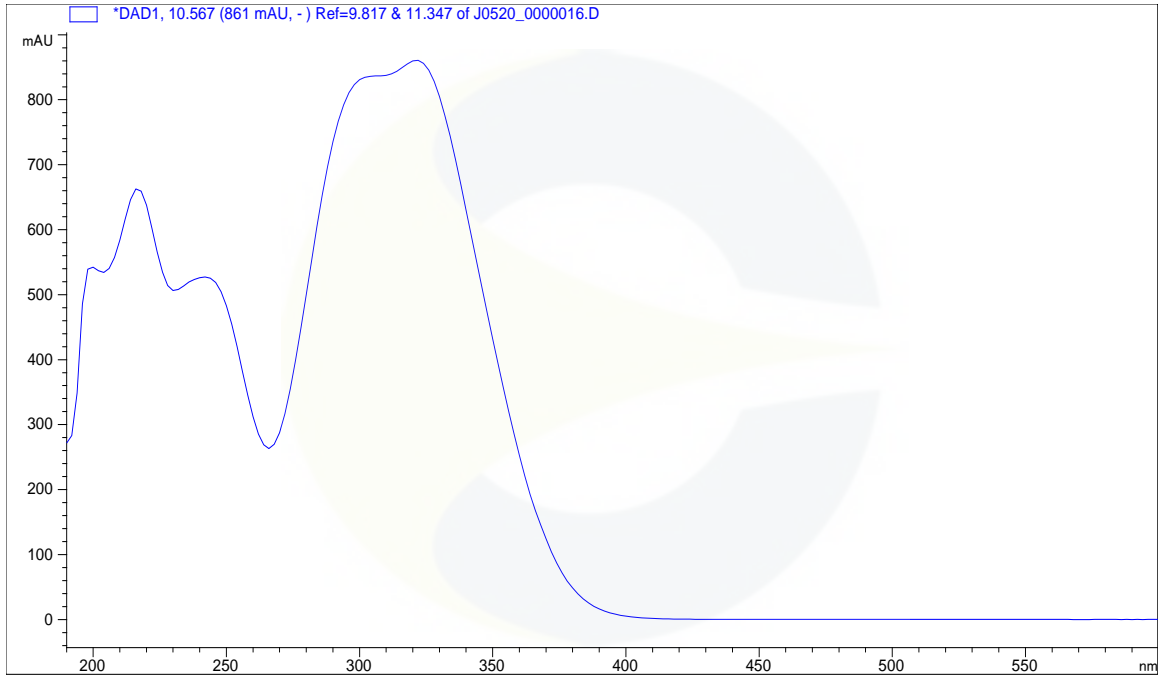
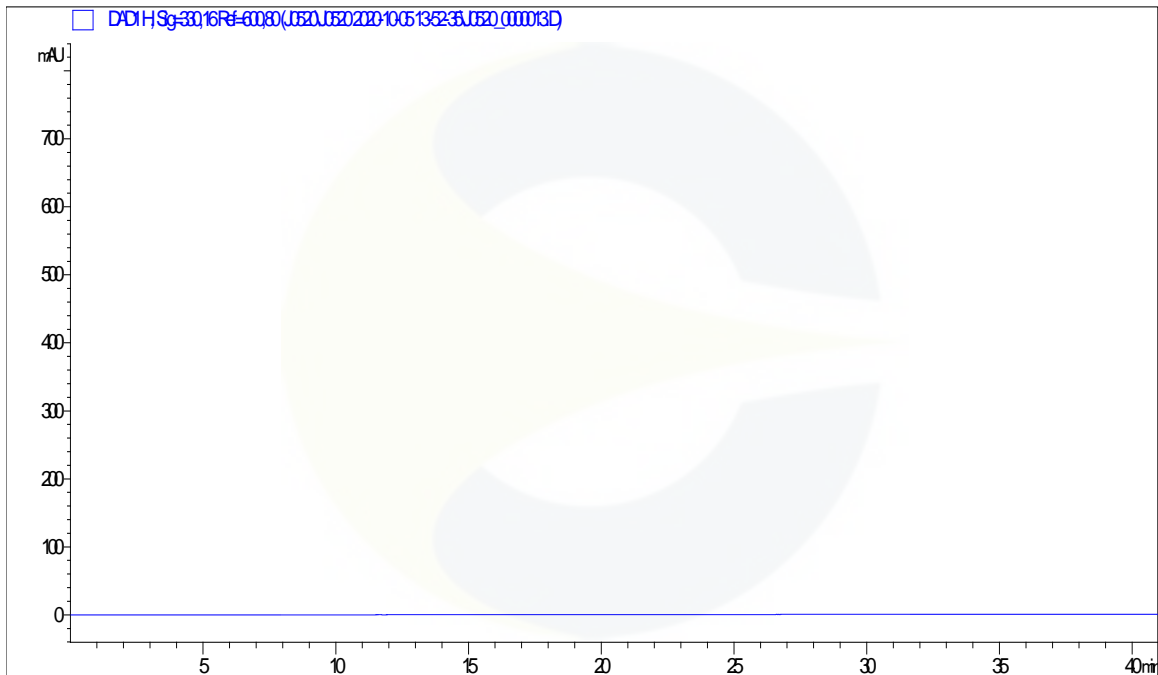
INSTRUMENT	AGILENT 1260 HPLC UV-VIS (DAD); AGILENT 1100 ION TRAP
COLUMN	Phenomenex Luna C18(2) 150 x 2.00 mm, 5 µm particle size
MOBILE PHASE	A - 0.1% Trifluoroacetic acid in Ultrapure water, B - Acetonitrile; Isocratic 5% B for 5 minutes, then increasing to 95% B over 20 minutes. Hold at 95% B for 15 minutes.
COLUMN TEMP.	60 °C
FLOW RATE	0.4 mL/minute
INJECTION VOL.	0.4 µL
INJECTION CONC.	1.0 mg/mL in Methanol
DETECTION	330 ± 8 nm

HPLC CHROMATOGRAM OF 1,3-DICAFFEOYLQUINIC ACID (CDXP-17-00265)



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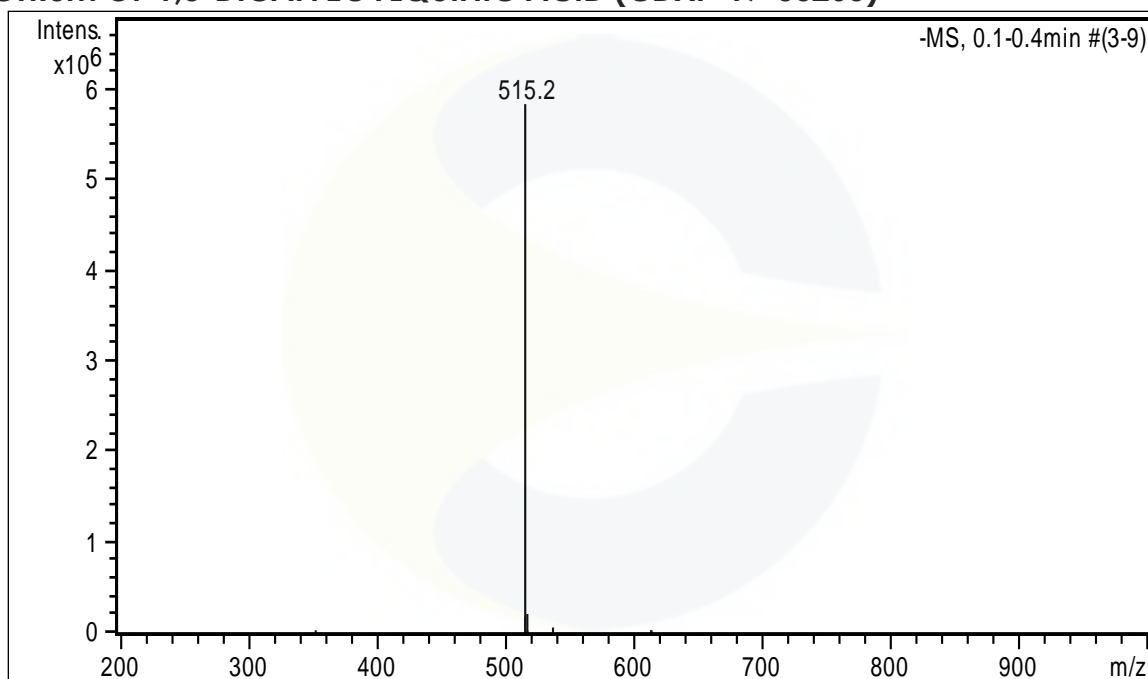
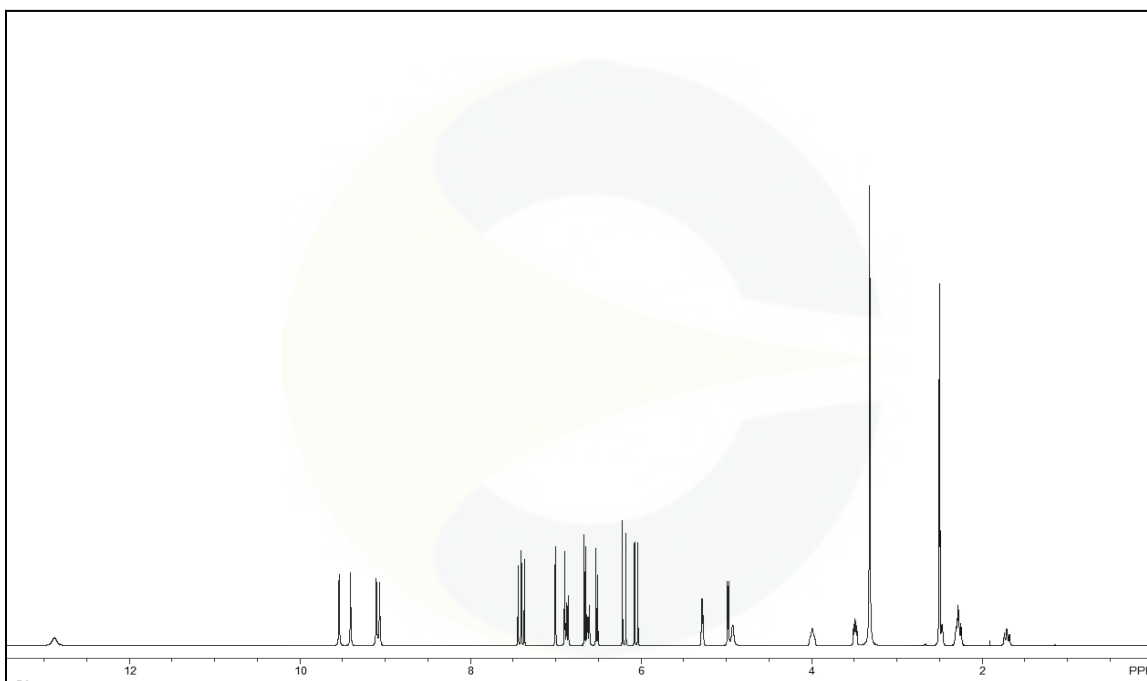
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UV SPECTRUM AT 10.6 MINUTES

HPLC CHROMATOGRAM OF DILUENT BLANK


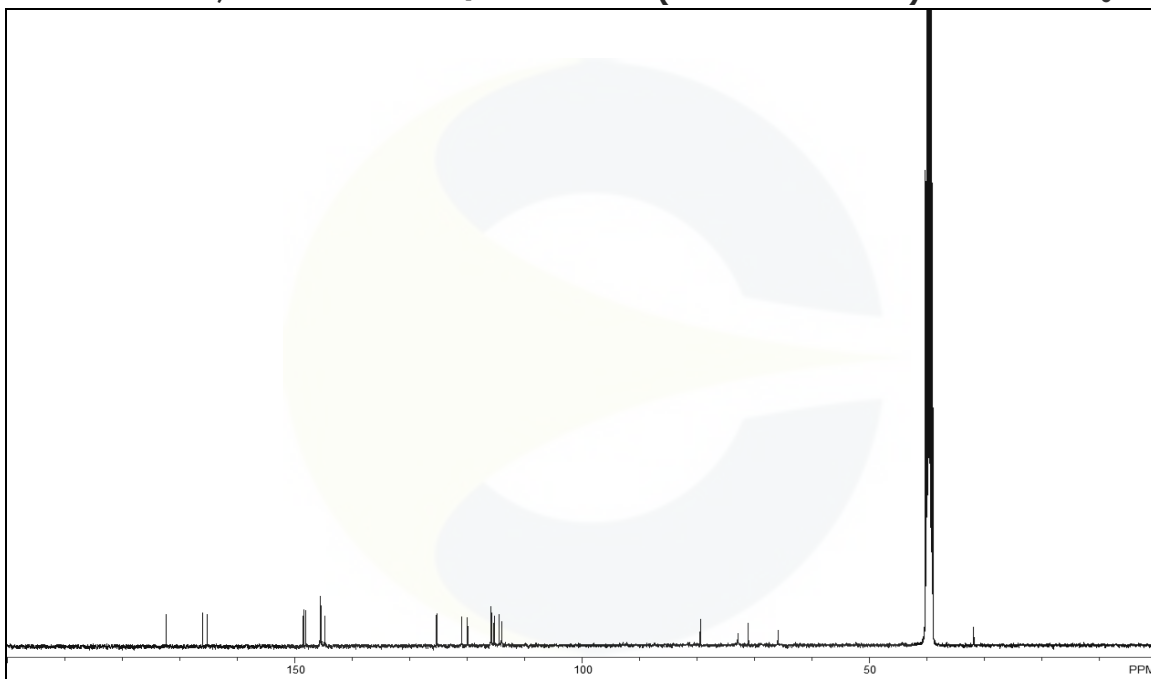
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MASS SPECTRUM OF 1,3-DICAFFEYOYLQUINIC ACID (CDXP-17-00265)

¹H-NMR SPECTRUM OF 1,3-DICAFFEYOYLQUINIC ACID (CDXP-17-00265) IN DMSO-d₆


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¹³C-NMR SPECTRUM OF 1,3-DICAFFEYLQUINIC ACID (CDXP-17-00265) IN DMSO-d₆

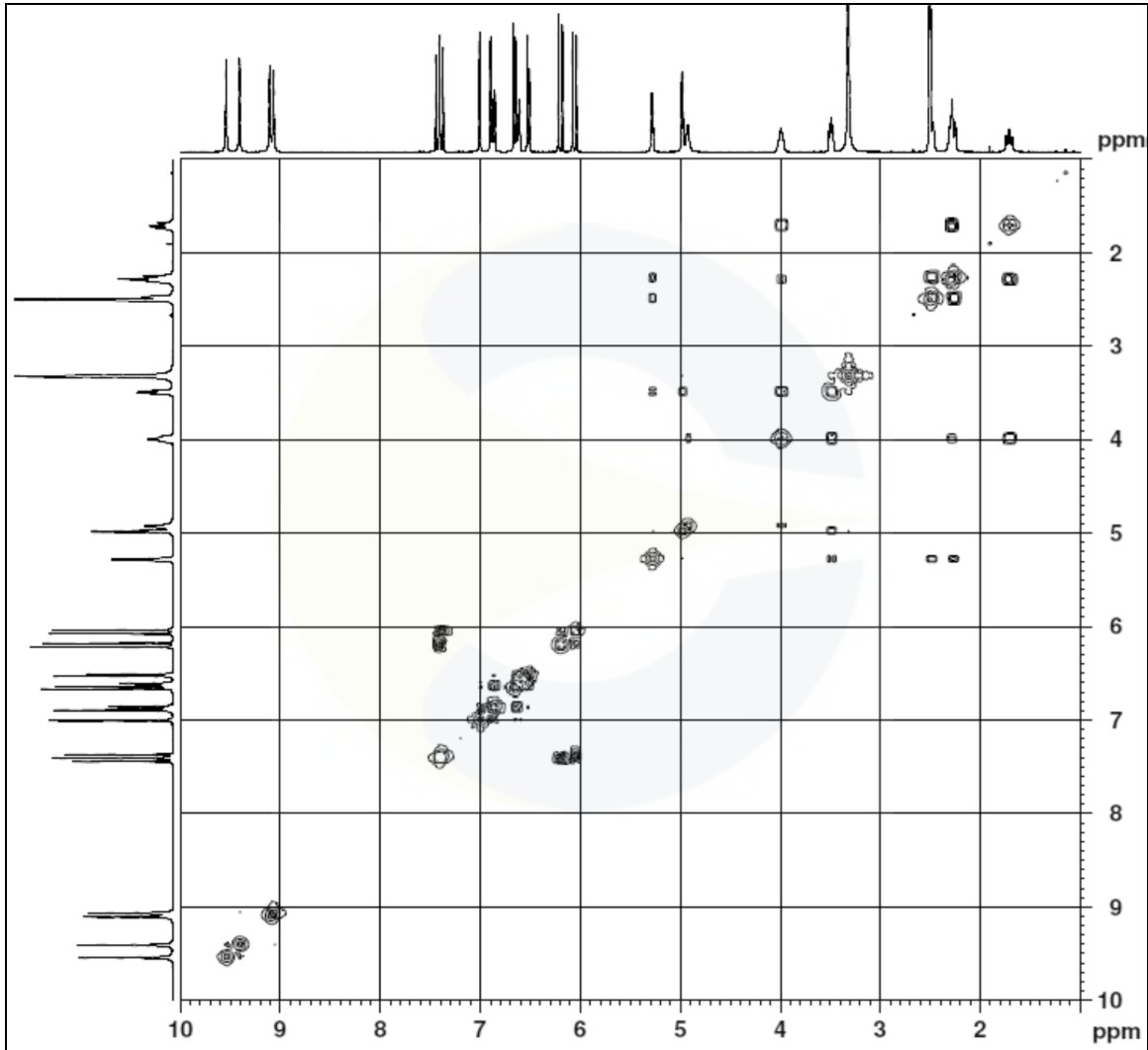
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COSY-NMR SPECTRUM OF 1,3-DICAFFEYOYLQUINIC ACID (CDXP-17-00265) IN DMSO-d₆



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REVISION HISTORY

<u>Revision History</u>	<u>Date of Revision</u>	<u>Document/Changes</u>
00	09/27/2016	New report
01	09/30/2016	Corrected Lot Number.
02	02/01/2018	Updated sample number, CAS number and chemical names. Removed melting point and instrument names.
03	12/04/2020	Passed re-evaluation by HPLC, KF, and NMR. Updated CAS number, analytical results, analytical conditions, chromatograms, and expiration date.
04	02/05/2021	Revision. Corrected CAS number and structure.

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