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**PRODUCT NAME** (-)-Gallocatechin

PART NUMBER 00007043

STANDARD TYPE Primary (P)

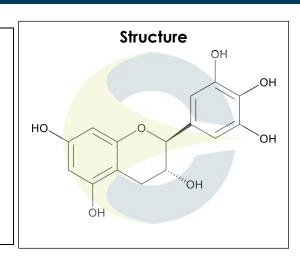
**LOT NUMBER** 00007043-306

REPORT NUMBER CDXA-RSS-9135-00

SAMPLE NUMBER CDXP-20-00633

**DATE OF SAMPLE** 08/26/2020

**DATE OF REPORT** 09/22/2020



CHEMICAL NAMES (2S,3R)-3,4-Dihydro-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3,5,7-triol

CHEMICAL FORMULA C<sub>15</sub>H<sub>14</sub>O<sub>7</sub>

MOLECULAR WEIGHT (MW) 306.27

CHEMICAL FAMILY Catechins

**CAS NUMBER** [3371-27-5]

**EC#(EINECS)** 608-899-7

RTECS N/A

### **ANALYTICAL RESULTS**

TEST	METHOD	SPECIFICATION	RESULT
Adjusted Purity	NA	≥ 85%	94.1%
HPLC	0.700.10.2.METH74	≥ 90%	99.9%
NMR	0.700.12.4	Conforms to structure	Conforms to structure
Mass Spectrum	0.700.12.27	Conforms	Conforms
Residual Solvent*	USP <467>	NA	ND
Water	0.700.12.37	NA	5.8%
Appearance	NA	NA	White powder

\*Testing performed at an ISO 17025 accredited subcontracted laboratory.

ADJUSTED PURITY: 94.1% IS BASED ON (100 - 0.0 SOLVENTS - 5.8 WATER) X 99.9% HPLC

#### STORAGE CONDITIONS

**STORAGE** +4 °C in a dry place.

**EXPIRATION DATE** 08/2025 under the above conditions.









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#### **ANALYTICAL CONDITIONS**

INSTRUMENT AGILENT 1290 UHPLC UV-VIS (DAD); AB-SCIEX 6600 TRIPLE TOF

**COLUMN** Phenomenex Kinetex Phenyl-Hexyl 50 x 2.1 mm, 2.6 µm particle size

MOBILE PHASE A – 97:2:1:0.1: Milli-Q:ACN:MeOH:Phosphoric acid, B – Methanol, C – Acetonitrile

Isocratic 100% A decreasing to 90% A and 10% B over 2 minutes, then

decreasing to 70% A and increasing to 15% B and 15% C, over 4 minutes, then hold at 70% A, decreasing to 10% B and increasing to 20% C, over 2 minutes. Decreasing to 60% A and 5% B and increasing to 35% C, over 4 minutes, then decreasing to 40% A, increasing to 10% B, and 50% C, over 0.5 minutes, then decreasing to 35% A, hold at 10% B, and increasing to 55% C, over 3 minutes.

Increasing to 100% A over 0.5 minutes. Hold at 100% A for 3 minutes.

**COLUMN TEMP.** 25 °C

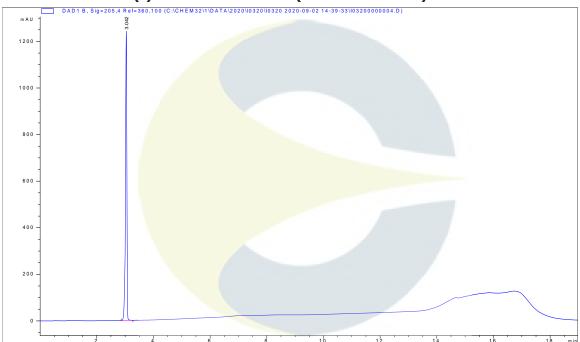
**FLOW RATE** 0.6 mL/minute

INJECTION VOL. 0.2 μL

**INJECTION CONC.** 1.2 mg/mL in Methanol

**DETECTION**  $205 \pm 2 \text{ nm}$ 

## HPLC CHROMATOGRAM OF (-)-GALLOCATECHIN (CDXP-20-00633)





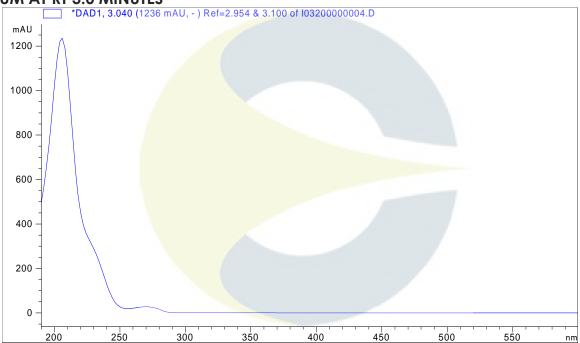




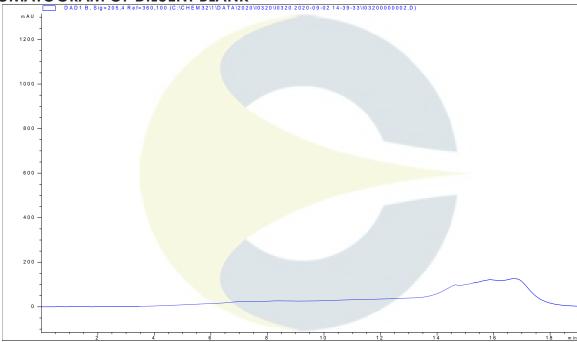


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#### **UV SPECTRUM AT RT 3.0 MINUTES**



#### HPLC CHROMATOGRAM OF DILUENT BLANK





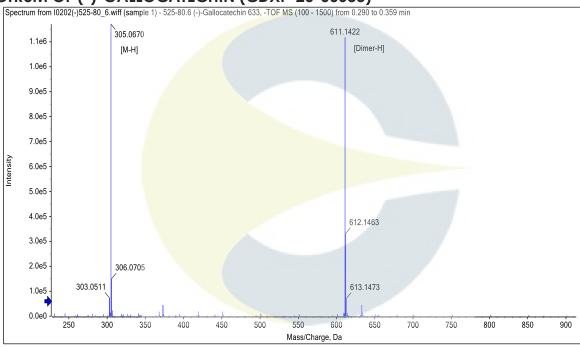




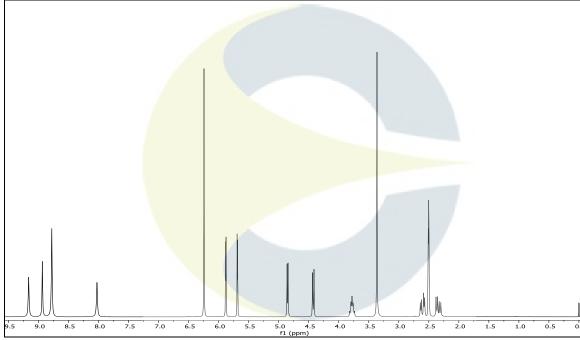


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### MASS SPECTRUM OF (-)-GALLOCATECHIN (CDXP-20-00633)









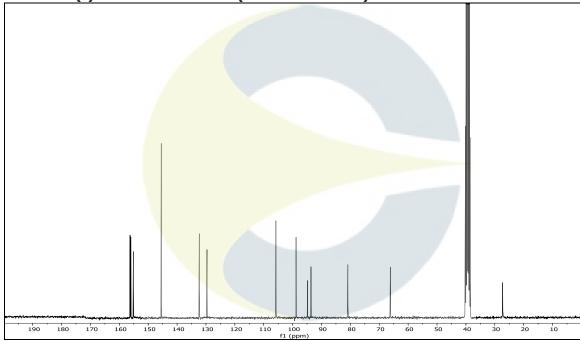






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13C-NMR SPECTRUM (-)-GALLOCATECHIN (CDXP-20-00633) IN DMSO-d6 + TMS





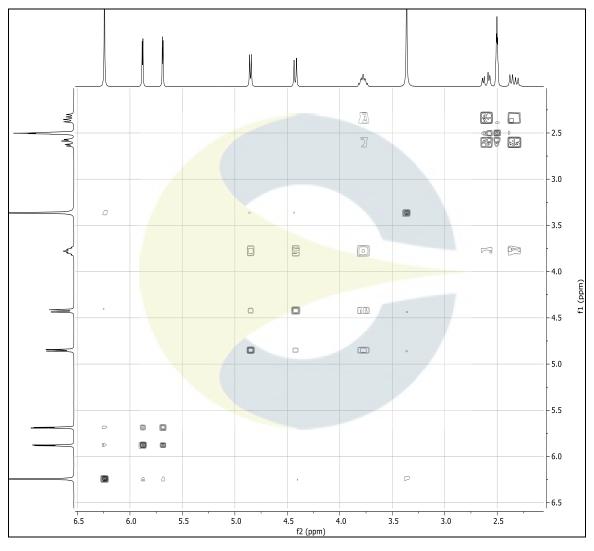






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## COSY-NMR SPECTRUM OF (-)-GALLOCATECHIN (CDXP-20-00633) IN DMSO-d6 + TMS



### **REVISION HISTORY**

**Revision History** Date of Revision **Document/Changes** 

00 09/22/2020 New report