





# Certificate of Analysis

For Laboratory Use Only

PRODUCT NAME Caffeic Acid

PART NUMBER 00003024

**STANDARD TYPE** Primary (P)

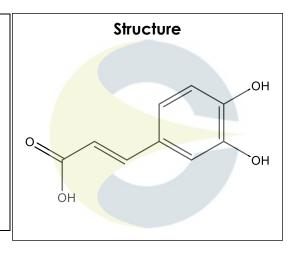
**LOT NUMBER** 00003024-O3L

REPORT NUMBER CDXA-RSS-10001-00

SAMPLE NUMBER CDXP-22-01038

**DATE OF SAMPLE** 11/04/2022

**DATE OF REPORT** 12/02/2022



CHEMICAL NAMES 3,4-Dihydroxybenzeneacrylic acid; 3-(3,4-Dihydroxyphenyl)-2-propenoic acid;

4-(2'-CarboxyvinyI)-1,2-dihydroxybenzene; 3,4-Dihydroxycinnamic acid

CHEMICAL FORMULA C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>

MOLECULAR WEIGHT (MW) 180.16

CHEMICAL FAMILY Phenolic Acids

**CAS NUMBER** [331-39-5]

**EC#(EINECS)** 206-361-2

**RTECS** GD8950000

#### **ANALYTICAL RESULTS**

| TEST              | METHOD            | SPECIFICATION         | RESULT                |
|-------------------|-------------------|-----------------------|-----------------------|
| Adjusted Purity   | NA                | ≥ 85%                 | 99.5%                 |
| HPLC              | 0.700.10.2.METH22 | ≥ 90%                 | 99.8%                 |
| NMR               | 0.700.12.4        | Conforms to structure | Conforms to structure |
| Mass Spectrum     | 0.700.12.27       | Conforms              | Conforms              |
| Residual Solvent* | USP <467>         | NA                    | Pyridine - 2630 ppm   |
| Water             | 0.700.12.37       | NA                    | ND                    |
| Appearance        | NA                | NA                    | Beige powder          |

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

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

#### STORAGE CONDITIONS

**STORAGE** Room Temperature in a dry place.







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**EXPIRATION DATE** 11/2027 under the above conditions.

### **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, then decreasing to 5% B over 1 minute.

COLUMN TEMP. 60 °C

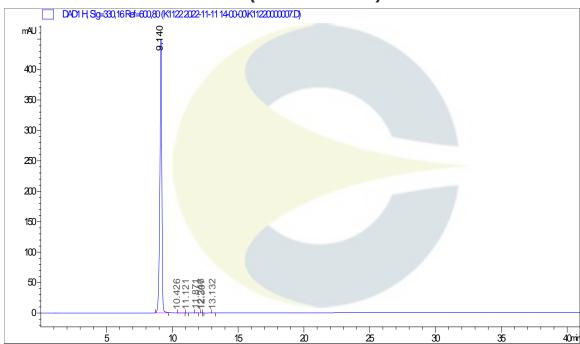
**FLOW RATE** 0.4 mL/minute

INJECTION VOL. 0.4 μL

**INJECTION CONC.** 1.0 mg/mL in Methanol

**DETECTION**  $330 \pm 8 \text{ nm}$ 

### HPLC CHROMATOGRAM OF CAFFEIC ACID (CDXP-22-01038)





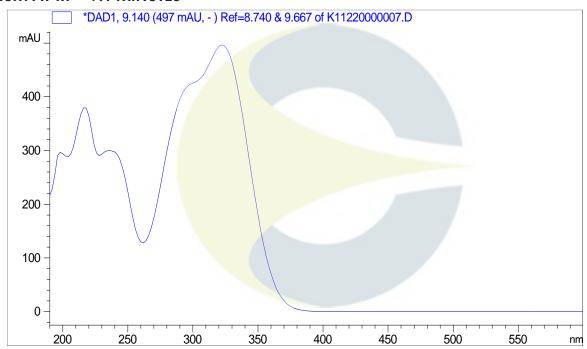




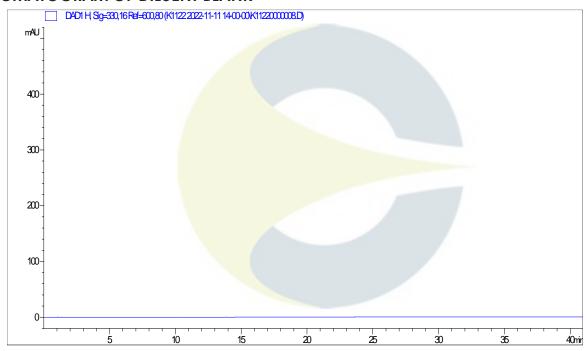
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#### **UV SPECTRUM AT RT = 9.1 MINUTES**



#### HPLC CHROMATOGRAM OF DILUENT BLANK





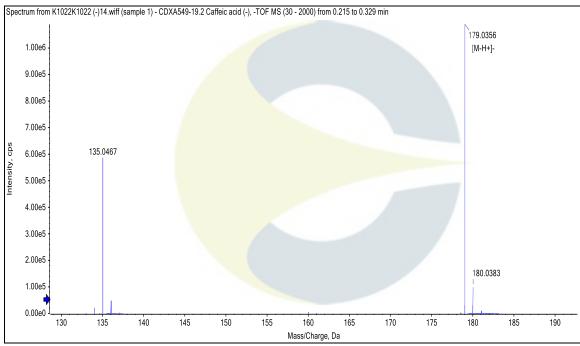




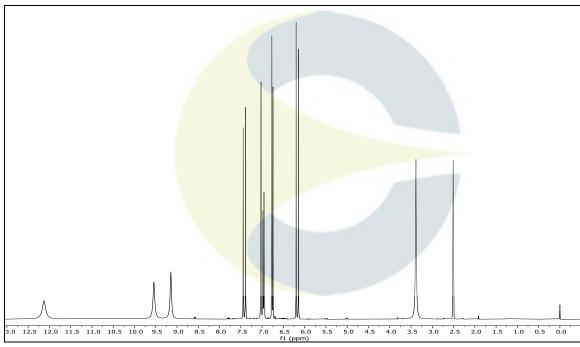
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### MASS SPECTRUM OF CAFFEIC ACID (CDXP-22-01038)



# <sup>1</sup>H-NMR SPECTRUM OF CAFFEIC ACID (CDXP-22-01038) IN DMSO-d<sub>6</sub> + TMS





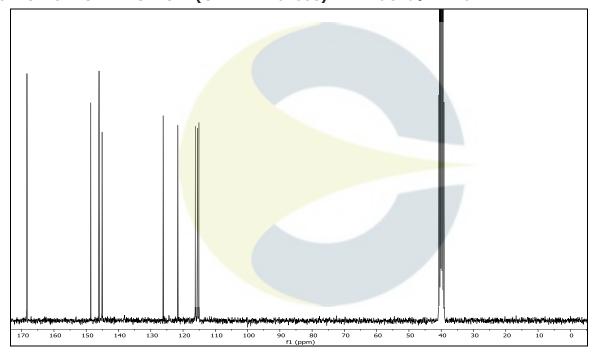




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## 13C-NMR SPECTRUM CAFFEIC ACID (CDXP-22-01038) IN DMSO-d6 + TMS





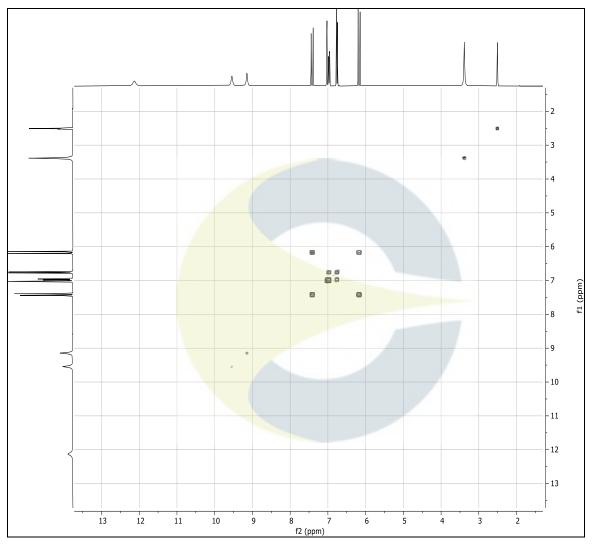




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## COSY-NMR SPECTRUM OF CAFFEIC ACID (CDXP-22-01038) IN DMSO-d6 + TMS



#### **REVISION HISTORY**

Revision History Date of Revision Document/Changes

00 12/02/2022 New report