ChromaDex CONNECTION

analytics consulting ingredients standards

Tech Tip 0001 - *Reference Standards Product Grades*

Choosing the correct reference standard is essential to the success of your quality management program or research project. ChromaDex offers three different product grades to suit your technical and budgetary needs. These product grades are differentiated by the level of characterization and testing performed and reported on the certificate of analysis. The below information will guide you in choosing the right product grade for your use. If you have any questions about our product grades or would like assistance in your choice, please let us know.

Primary Analytical Standards (P)

Primary Standards are orthogonally characterized by multiple analytical techniques. These products include a complete certificate of analysis for each lot that lists adjusted (as-is) purity calculated by HPLC or GC chromatographic purity, Karl Fischer (water content), and GC (residual solvent). The identity of these standards is confirmed with Mass Spectrometry and NMR. The certificate of analysis includes analytical conditions, chromatograms, and spectra for your reference, allowing you to replicate the tests in your laboratory. When utilizing a reference standard for quantitative analysis, the best choice is a Primary Standard.

Analytical Standards (AS)

Analytical Standard grade is a step below our Primary grade regarding the level of characterization reported on the certificate of analysis accompanying each lot. The purity of these products is determined by HPLC or GC chromatographic purity. Identity is confirmed by one technique, typically Mass Spectrometry. Water and residual solvent content are not reported for Analytical Standards.

Reagent Grade Chemicals (RG)

Reagent Grade Chemicals are suitable as fine chemicals for many laboratories. However, they are not intended for use as reference standards. The certificate of analysis for RG chemicals contains basic physical properties, but the materials are not characterized for purity. As a result, RG chemicals are not suitable for direct quantitative use.

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Tech Tip 0001 - *Reference Standards Product Grades*

ChromaDex product grades are differentiated by the level of characterization and testing performed and reported for each lot of material.

Grade	Chemical Data	Adjusted Purity	HPLC/ GC %	Water %	Solvent %	NMR	Mass Spec
Primary Analytical Standard (P)	✓	✓	✓	✓	✓	✓	✓
Analytical Standard* (AS)	✓		✓				✓
Reagent Grade (RG)	✓						

Depending on your project and needs, different end uses require different product grades. Here is an overview of some typical uses and appropriate ChromaDex product grades for each.

Grade	Quantitative HPLC/GC	Quality Control	Method Devel.	Working Stnd.	Cell Assays	Basic Research
Primary Analytical Standard (P)	✓	✓	✓	✓	✓	✓
Analytical Standard (AS)	✓*	✓*	✓	✓	✓	✓
Reagent Grade (RG)					✓	✓

*Since Analytical Standard (AS) grade products are not corrected for water and solvent content, quantitative results from these standards will give content on chromatographic purity only and will not account for the water and solvent that is contained in the sample being tested. Whenever possible for the most accurate analytical results, the best choice for quantitative analysis is a Primary Analytical Standard (P).

In addition to our three product grades, ChromaDex offers two additional specialized types of Primary Standards. These products are full Primary Standards with additional value-added testing and results.

Primary Certified Reference Material (CRM)

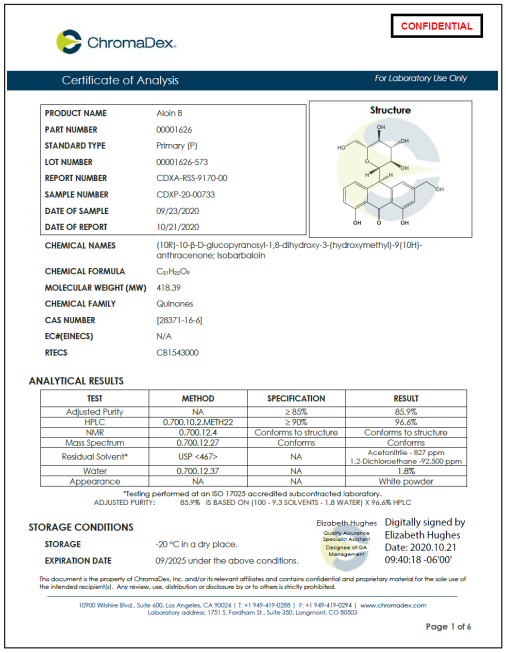
For increased compliance if your laboratory is ISO accredited, ChromaDex produces select Primary Standards in accordance with our ISO 17034 Certified Reference Material Producer and ISO/IEC 17025 Chemical Testing Laboratory accreditations. Our Primary CRMs are the most rigorously tested materials in our catalogue, providing the best accuracy and most thorough certificates of analysis. In addition to the full Primary characterization, these materials include a reported uncertainty value for the HPLC or GC chromatographic purity. This overall value incorporates the uncertainty of the test method analysis, sample homogeneity, stability, and transport. The extra reported information will allow your laboratory to properly calculate measurement uncertainty for your sample analyses.

Compendial Traceable Primary Analytical Standards (CT)

As an added value to our clients, ChromaDex is now offering Primary Analytical Standards (P) that are also traceable to a compendial reference material. These products undergo full Primary characterization and also have a purity assay value tested against a compendial material such as supplied by the United States Pharmacopeia (USP), National Institute of Standards and Technology (NIST), or other similar international compendial. Certificates of Analysis for these products include full data for Primary Analytical Standards along with a listing of the compendial source, lot number, and assay value.

Tech Tip 0001 - *Reference Standards Product Grades*

Example: Primary Grade Certificate of Analysis



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Certificate of Analysis — For Laboratory Use Only

PRODUCT NAME	Aloin B
PART NUMBER	00001626
STANDARD TYPE	Primary (P)
LOT NUMBER	00001626-573
REPORT NUMBER	CDXA-RSS-9170-00
SAMPLE NUMBER	CDXP-20-00733
DATE OF SAMPLE	09/23/2020
DATE OF REPORT	10/21/2020

Structure

CHEMICAL NAMES	(10R)-10-β-D-glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10H)-anthracenone; Isobarbaloin
CHEMICAL FORMULA	$C_{21}H_{22}O_9$
MOLECULAR WEIGHT (MW)	418.39
CHEMICAL FAMILY	Quinones
CAS NUMBER	[28371-16-6]
EC#(EINECS)	N/A
RTECS	CB1543000

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT
Adjusted Purity	NA	≥ 85%	85.9%
HPLC	0.700.10.2.METH22	≥ 90%	96.6%
NMR	0.700.12.4	Conforms to structure	Conforms to structure
Mass Spectrum	0.700.12.27	Conforms	Conforms
Residual Solvent*	USP <467>	NA	Acetonitrile - 827 ppm 1,2-Dichloroethane -92.500 ppm
Water	0.700.12.37	NA	1.8%
Appearance	NA	NA	White powder

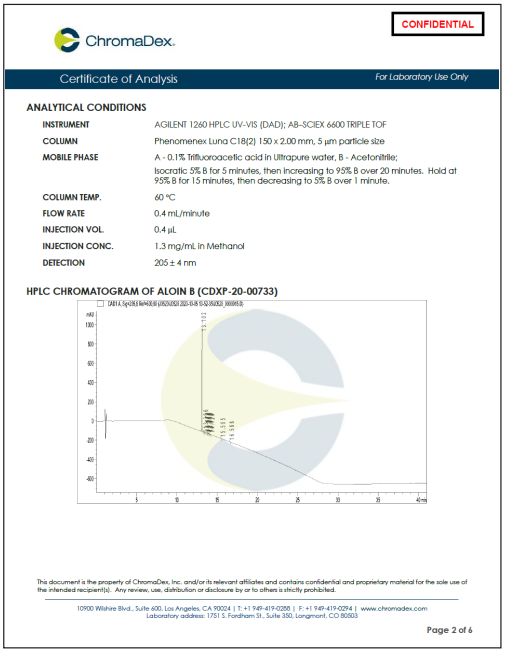
*Testing performed at an ISO 17025 accredited subcontracted laboratory.
ADJUSTED PURITY: 85.9% IS BASED ON (100 - 9.3 SOLVENTS - 1.8 WATER) X 96.6% HPLC

STORAGE CONDITIONS

STORAGE	-20 °C in a dry place.
EXPIRATION DATE	09/2025 under the above conditions.

Elizabeth Hughes, Quality Assurance Specialist Assistant, Designee of QA Management

Digitally signed by Elizabeth Hughes
Date: 2020.10.21 09:40:18 -06'00'



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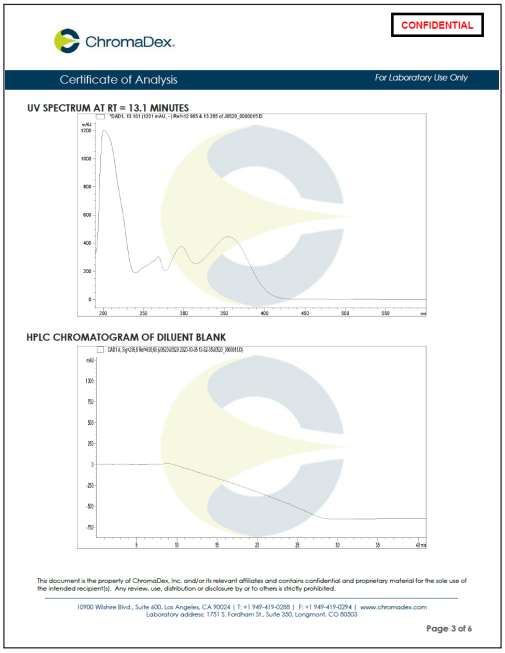
ANALYTICAL CONDITIONS

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, 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.	1.3 mg/mL in Methanol
DETECTION	205 ± 4 nm

HPLC CHROMATOGRAM OF ALOIN B (CDXP-20-00733)



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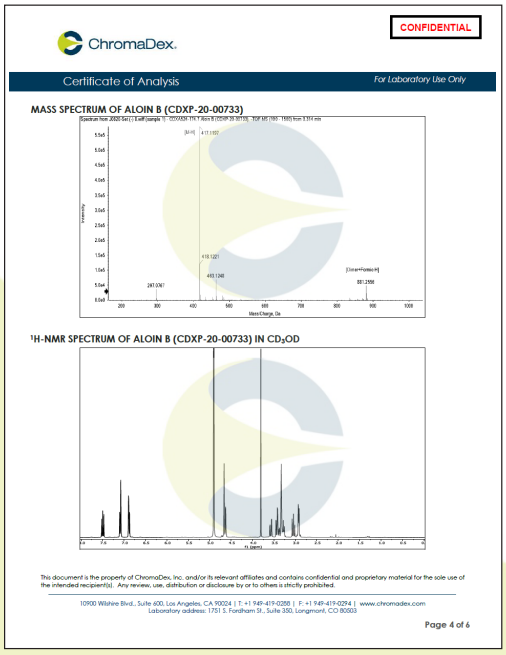
UV SPECTRUM AT RT = 13.1 MINUTES

HPLC CHROMATOGRAM OF DILUENT BLANK



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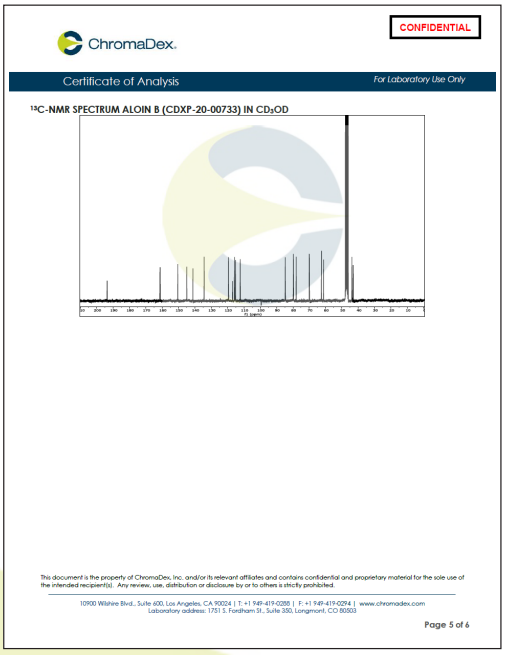
MASS SPECTRUM OF ALOIN B (CDXP-20-00733)

^{1}H-NMR SPECTRUM OF ALOIN B (CDXP-20-00733) IN CD_3OD



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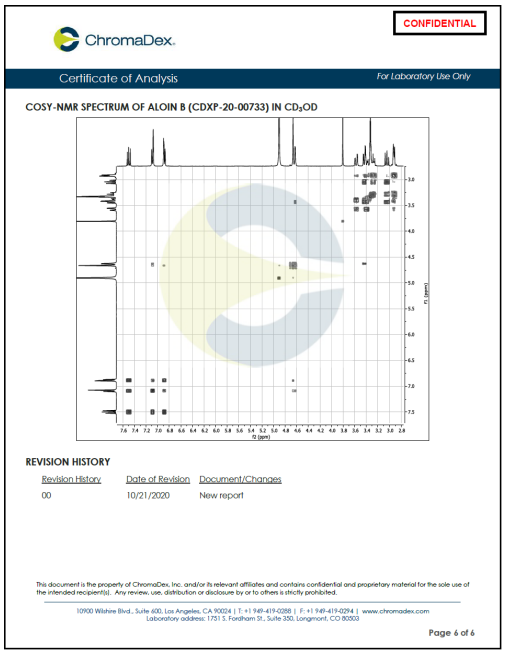
^{13}C-NMR SPECTRUM ALOIN B (CDXP-20-00733) IN CD_3OD



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COSY-NMR SPECTRUM OF ALOIN B (CDXP-20-00733) IN CD_3OD

REVISION HISTORY

Revision History	Date of Revision	Document/Changes
00	10/21/2020	New report

Tech Tip 0001 - *Reference Standards Product Grades*

Example: Analytical Standard Grade Certificate of Analysis

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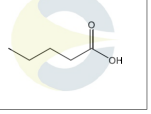
Certificate of Analysis — *For Laboratory Use Only*

PRODUCT NAME	Valeric acid
PART NUMBER	00022195
STANDARD TYPE	Analytical Standard (AS)
LOT NUMBER	00022195-WKF
REPORT NUMBER	CDXA-RSS-7454-01
SAMPLE NUMBER	CDXA-17-000507
DATE OF SAMPLE	01/11/2017
DATE OF RE-EVALUATION	03/05/2021
DATE OF REPORT	03/31/2021

Structure



CHEMICAL NAMES	1-Butanecarboxylic acid; n-Pentanoic acid; Pentanoic acid; Propylacetic acid
CHEMICAL FORMULA	$C_5H_{10}O_2$
MOLECULAR WEIGHT (MW)	102.13
CHEMICAL FAMILY	Oils
CAS NUMBER	[109-52-4]
EC#(EINECS)	203-677-2
RTECS	YV6100000

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT
GC	0.700.10.2.METH140	≥ 75%	99.2%
Mass Spectrum	0.700.10.2.METH140	Conforms	Conforms
Appearance	NA	NA	Liquid

STORAGE CONDITIONS

STORAGE	+4 °C in a dry place.
EXPIRATION DATE	03/2026 under the above conditions.

Elizabeth Hughes Quality Assurance Specialist

Digitally signed by Elizabeth Hughes
Date: 2021.03.31 16:01:26 -06'00'

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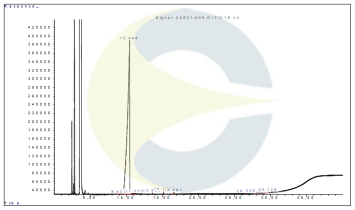
ANALYTICAL CONDITIONS

INSTRUMENT	AGILENT 7890B WITH FLAME IONIZATION DETECTOR (FID) AND AGILENT 5977B MASS SELECTIVE DETECTOR (MSD)
COLUMN	Phenomenex Zebron ZB-5plus, 30 m x 0.32 mm x 0.25 µm
CARRIER GAS	Helium
COLUMN TEMP.	Isothermic 40 °C for 5.0 minutes, then increasing at 10.0 °C/minute to 340 °C. Hold at 340 °C for 5.0 minutes.
FLOW RATE	2.0 mL/minute
INJECTOR TEMP.	300 °C
INJECTOR SPLIT RATIO	20:1
INJECTION VOL.	1.0 µL
INJECTION CONC.	1.9 mg/mL in Chloroform
DETECTION	FID (350 °C) & MSD (Transfer line 280 °C, Source 230 °C, Quad 150 °C)

GC CHROMATOGRAM OF VALERIC ACID (CDXA-17-000507)



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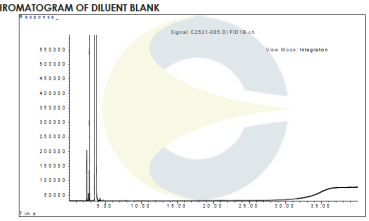
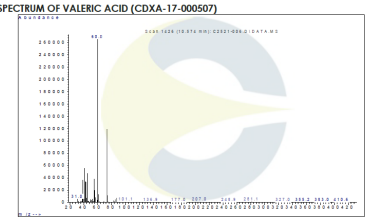
GC CHROMATOGRAM OF DILUENT BLANK



MASS SPECTRUM OF VALERIC ACID (CDXA-17-000507)



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REVISION HISTORY

Revision History	Date of Revision	Document/Changes
00	03/09/2017	New report
01	03/31/2021	Material passed reeval by GC-MS. Updated analytical results, analytical conditions, chromatograms, spectrum, and expiration date. Removed melting point.

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Example: Reagent Grade Certificate of Analysis

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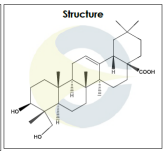
Certificate of Analysis — *For Laboratory Use Only*

PRODUCT NAME	Hederagenin
PART NUMBER	00008067
STANDARD TYPE	Reagent grade (RG)
LOT NUMBER	00008067-B15
REPORT NUMBER	CDXA-RSS-7202-01
SAMPLE NUMBER	CDXP-21-00204
DATE OF SAMPLE	07/13/2016
DATE OF RE-EVALUATION	03/25/2021
DATE OF REPORT	04/01/2021

Structure



CHEMICAL NAMES	(3β,4α)-3,23-Dihydroxyolean-12-en-28-oic acid; Astrantiagenin E; Caulosapogenin; Hederagenic acid; Hederagenol
CHEMICAL FORMULA	$C_{30}H_{48}O_4$
MOLECULAR WEIGHT (MW)	472.70
CHEMICAL FAMILY	Triterpenes
CAS NUMBER	[465-99-6]
EC#(EINECS)	207-369-9
RTECS	RK0177850

STORAGE CONDITIONS

STORAGE	Room Temperature in a dry place.
EXPIRATION DATE	03/2026 under the above conditions.

Elizabeth Hughes Quality Assurance Specialist

Digitally signed by Elizabeth Hughes
Date: 2021.04.01 16:15:57 -06'00'

REVISION HISTORY

Revision History	Date of Revision	Document/Changes
00	08/03/2016	New report
01	04/01/2021	Passed re-evaluation by MS. Updated expiration date and removed melting point.

Note – Reagent Grade (RG) chemicals are not guaranteed as quantitative standards. This product line has been developed for research and qualitative purposes only.

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