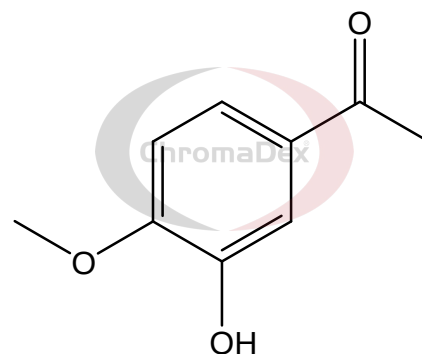


PRODUCT	Acetoisovanillone
PART NUMBER	00001079
STANDARD TYPE	Secondary (SH)
LOT NUMBER	00001079-631
REPORT NUMBER	CDXA-RSS-4913-00
CDXA NUMBER	CDXA-12-1019
DATE OF SAMPLE	02/28/2012
DATE OF REPORT	03/29/2012

Structure


NAME	Acetoisovanillone
OTHER NAME	1-(3-Hydroxy-4-methoxyphenyl)-ethanone
CHEMICAL FORMULA	C ₉ H ₁₀ O ₃
MOLECULAR WEIGHT (MW)	166.17
PUBLISHED MELTING POINT	NA
CAS NUMBER	[6100-74-9]
EINECS	NA
CHEMICAL FAMILY	Phenolic acids
RTECS	NA

ANALYTICAL RESULTS

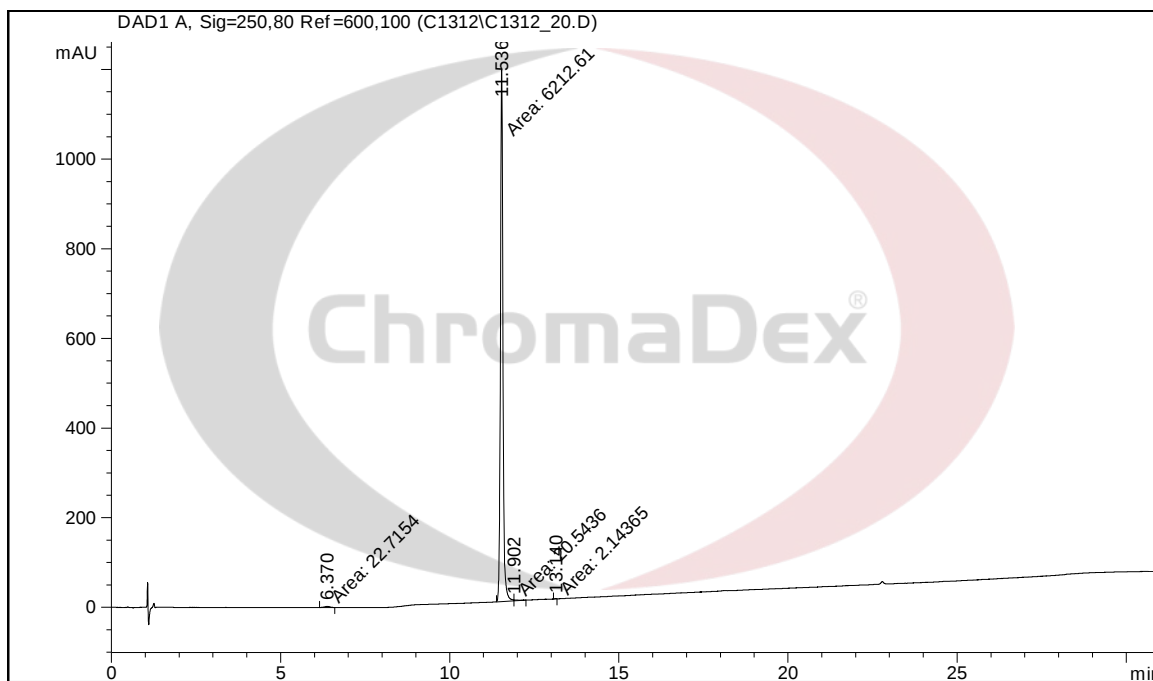
TEST	METHOD	SPECIFICATION	RESULT
HPLC	See below	NA	99.3%
Mass Spectrum	Direct Infusion, ESI (+)	Conforms	Conforms
Appearance	NA	NA	White powder

STORAGE CONDITIONS

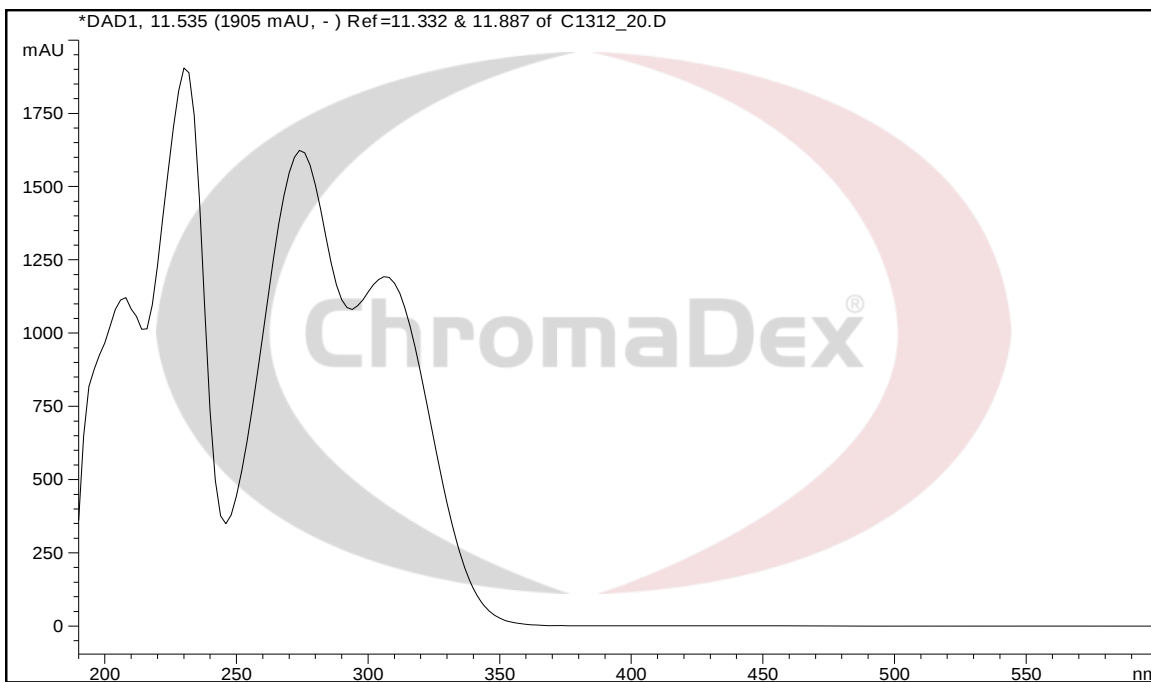
STORAGE	Room Temperature in a dry place.
EXPIRATION DATE	02/2017 under the above conditions.

ANALYTICAL CONDITIONS

INSTRUMENT	AGILENT 1100 HPLC UV-VIS (DAD) DETECTOR (YOUNG), AGILENT 6510 QTOF (AVOGADRO)
COLUMN	Phenomenex Luna C18(2) 150 x 2.00 mm, 5 µm particle size; S/N 573498-6
MOBILE PHASE	A - 0.1% Formic acid in Milli-Q water, B – 0.1% Formic acid in Acetonitrile; Isocratic 5% B for 5 minutes, then increasing to 95% B over 20 minutes. Hold at 95% B for 5 minutes.
COLUMN TEMP.	60°C
FLOW RATE	0.4 mL/minute
INJECTION VOL.	0.2 µL
INJECTION CONC.	3.6 mg/mL in Methanol
DETECTION	250 ± 40 nm

HPLC CHROMATOGRAM OF ACETOISOVANILLONE (CDXA-12-1019)

UV SPECTRUM AT RT = 11.5 MINUTES



MASS SPECTRUM OF ACETOISOVANILLONE (CDXA-12-1019)

