



REFERENCE MATERIAL ANALYSIS REPORT

Report ID: D468.2011.03

Compound Name: *trans*-Cinnamoyl cocaine

Collection No: D468

Chemical Formula: C₁₉H₂₃NO₄

CAS No: 50763-20-7

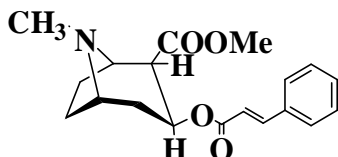
Structure:

Description: White powder

Batch No: 96-11201

Molecular Weight: 329.3

Batch production completed: March 1997



Synonyms: (E)-[1R-(*exo,exo*)]-8-Methyl-3-[(1-oxo-3-phenyl-2-propenyl)oxy]-8-azabicyclo[3,2,1]-octane-2-carboxylic acid methyl ester
Ecgonine cinnamate methyl ester
Cinnamoylcocainmethyl ester
Cinnamoylmethylecgonine

Purity (mass fraction): 98.2 ± 0.5% (95% coverage interval)

Purity estimate obtained by subtraction from 100% of total impurities by GC-FID and TGA analysis.

GC-FID Instrument: Agilent 6890N
Column: HP-1, 29.93 m × 0.32 mm × 0.25 μm
Program: 160 °C (1 min), 10 °C/min to 250 °C (4 min), 30 °C/min to 300 °C (3 min)
Injector: 250 °C Detector Temp: 300 °C
Carrier: Helium Split ratio: 20/1
Relative peak area response of main component:
Initial analysis: Mean > 99.9%, (7 sub samples, February 1997)
Current re-analysis: Mean = 99.0%, s = 0.03 (5 sub samples in duplicate, February 2011)

GC-MS: Instrument: HP 6890 / 5973
Column: HP-Ultra 2 capillary, 12 m x 0.22 mm x 0.1 μm
Program: 70 °C, 10 °C/min to 300 °C, hold 4 min
Injector: 280 °C Transfer line temp: 280 °C
Carrier: Helium, 1.0 mL/min Split ratio: 10/1
The retention time is reported along with the major peaks in the mass spectrum.
The latter are reported in mass / charge ratios (in brackets) as a percentage relative to the base peak.
12.8 min: 329 (M⁺, 6), 238 (10), 131 (26), 103 (27), 96 (46), 94 (41), 82 (100) m/z

TLC: Conditions: Kieselgel 60F₂₅₄. Cyclohexane/toluene/diethylamine (75/15/10).
Single spot observed, R_f = 0.38 (visualisation with UV-light at 254 nm)

IR: Instrument: BioRad FTS3000MX FT-IR
Range: 4000-400 cm⁻¹, KBr powder
Peaks: 2959, 2856, 2804, 1749, 1699, 1630, 1319, 1179, 1037, 1008, 767, 683 cm⁻¹

Accredited for compliance with ISO Guide 34.

105 Delhi Road North Ryde NSW 2113 PO Box 138 North Ryde NSW 1670 Tel: +61 2 9449 0111 www.measurement.gov.au ABN: 74 599 608 295

Melting point: 121 °C

Thermogravimetric analysis: Volatile content 0.8 % total mass fraction. Non-volatile residue < 0.2 % mass fraction. (March 2006 & March 2011)

Karl Fischer analysis: Moisture content <0.1% mass fraction (February 2011).

Expiration of certification

The property values are valid till 25th February 2016, i.e. five years from the date of re-certification provided the **unopened** material is handled and stored in accordance with the recommendations below. The material as issued in the unopened container and stored as recommended below should be suitable for use beyond this date, subject to confirmation of batch stability from the issuing body.

The expiry date/shelf life does not apply to sample bottles/ampoules that have been opened. In such cases it is recommended that the end-user conduct their own in-house stability trials.

The long-term stability of the compound in solution has not been examined.

This material has demonstrated stability over a minimum period of 5 years. The measurement uncertainty at the 95% confidence interval includes a stability component which has been estimated from annual stability trials.

Recommended storage

When not in use this material should be stored at or below 4 °C in a closed container in a dry, dark area.

Intended Use

For *in vitro* laboratory analysis only.

Caution

Treat as hazardous substance. Use appropriate work practices when handling to avoid skin or eye contact, ingestion or inhalation of dust.

Legal notice

Neither NMI nor any person acting on NMI's behalf assumes any liability with respect to the use of, or for damages resulting from the use of, this reference material or the information contained in this certificate.

Authorised by:

S. R. Davies

Dr Stephen R Davies
Team Leader,
Chemical Reference Materials, NMI.
Dated: 16 April, 2014.

Characterisation data and property values specified in this report supersede those in all reports issued prior to 16 April, 2014.



Accredited for compliance with ISO Guide 34.

105 Delhi Road North Ryde NSW 2113 PO Box 138 North Ryde NSW 1670 Tel:+61 2 9449 0111 www.measurement.gov.au ABN: 74 599 608 295