

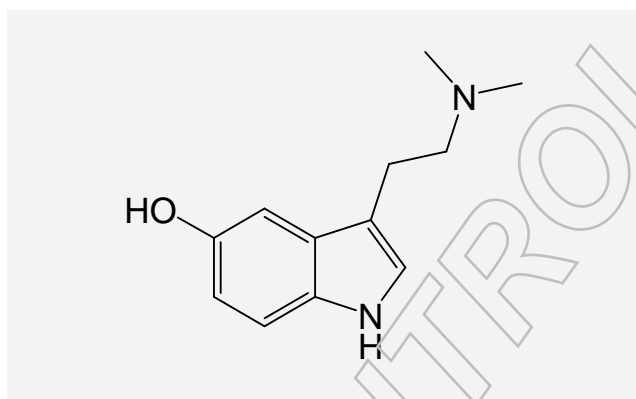
Certificate of Analysis

Reference Substance

Bufotenine

Catalogue Number: LGCFOR1360.10
Lot Number: 17217
Molecular Formula: C₁₂H₁₆N₂O
Molecular Weight: 204.27
CAS Number: [487-93-4]

Long-term Storage: 2 to 8 °C, dark
Appearance: beige solid
Melting Point: 88 °C
hygroscopic
Assay 'as is': 95.1 %




Date of shipment: **2016-May-20**

This certificate is valid for two years from the date of shipment provided the substance is stored under the recommended conditions.

Release Date: 2012-07-16

LGC GmbH



Dr. Sabine Schröder

Product Release

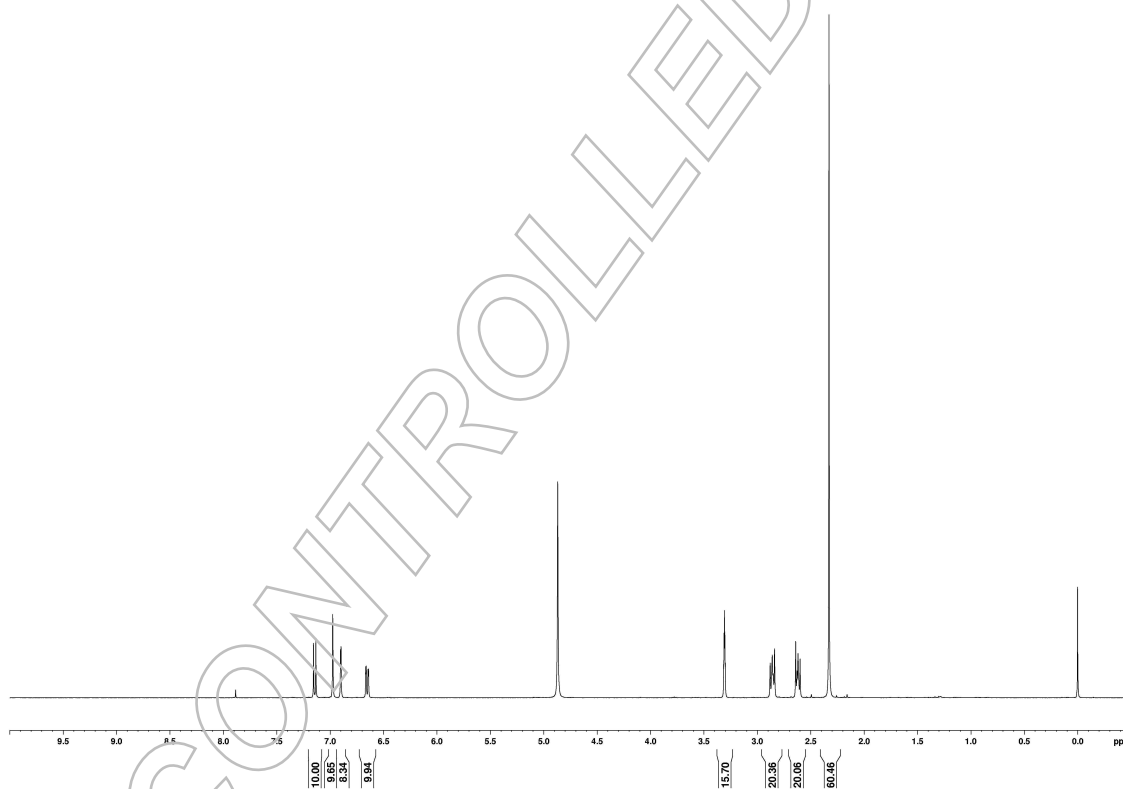
I. Identity

The identity of the reference substance was established by following analyses.

Ia. ¹H-NMR Spectrum

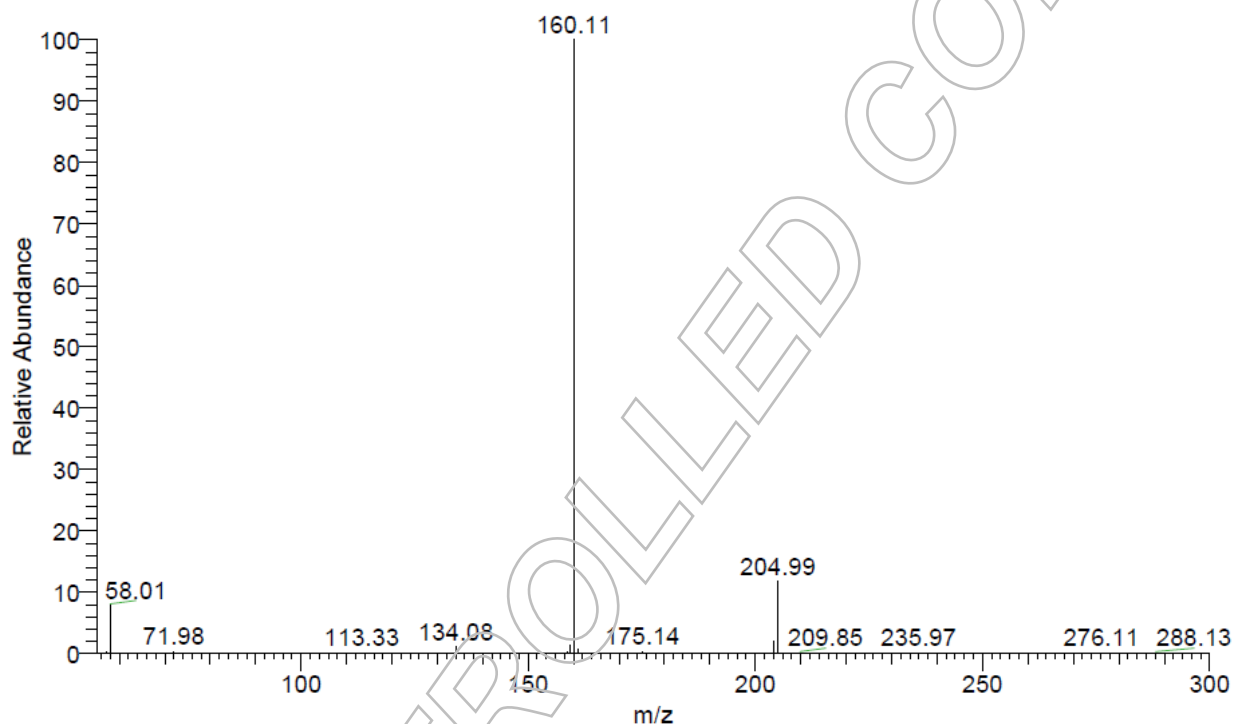
Conditions: 400 MHz, CD₃OD

The structure is confirmed with the signals of the spectrum and their interpretation.



1b. Mass Spectrum

Method: 4.5 kV ESI; vaporization temperature: 200 °C, direct inlet

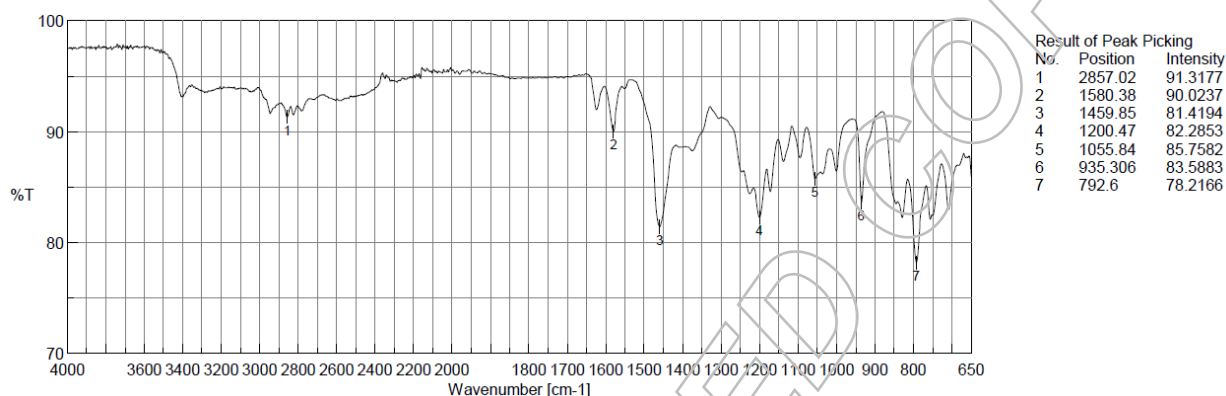


m/z	fragments
205	[MH]
160	[M – N(CH ₃) ₂]

The signals of the mass spectrum and their interpretation are consistent with the structural formula.

Ic. IR Spectrum

Method: Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) Spectroscopy



The signals of the IR spectrum and their interpretation are consistent with the structural formula.

II. Purity

The purity of the reference substance was analysed by high performance liquid chromatography (HPLC).

HPLC Conditions:

Column:

Hypersil Gold (C18)
5 µm, 150 x 4.6 mm

Conditions:

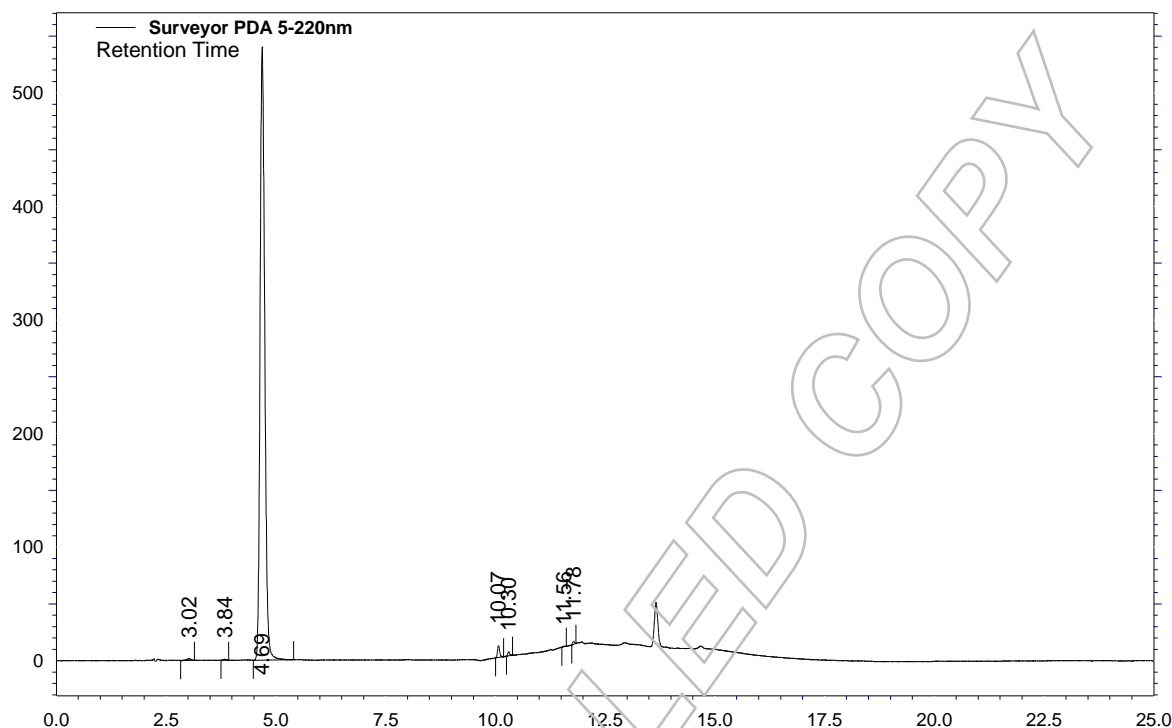
1.0 ml/min, 40 °C
0 – 6 min Water/Acetonitrile 98/2
6 – 9 min Water/Acetonitrile to 50/50
9 – 12 min Water/Acetonitrile 50/50
12 – 15 min Water/Acetonitrile to 98/2
15 – 25 min Water/Acetonitrile 98/2 (v/v);
0.1 % H₃PO₄

Detector:

DAD
220 nm

Injector:

Auto
0.5 µl; 0.3636 mg/ml in
Acetonitrile



Area Percent Report - Sorted by Signal

Pk #	Retention Time	Area	Area %
1	3.02	11199	0.28
2	3.84	3602	0.09
3	4.69	3995150	98.29
4	10.07	35293	0.87
5	10.30	10463	0.26
6	11.56	1590	0.04
7	11.78	7361	0.18
Totals		4064658	100.00

For the calculation the system peaks were ignored. The content of the analyte was determined as ratio of the peak area of the analyte and the cumulative areas of the purities, added up to 100 %.

Results:

Average 98.29 %
Number of results n=3
Standard deviation < 0.01 %

III. Water Content

Method: Karl Fischer titration

Results:

Average	0.30 %
Number of results	n=3
Standard deviation	0.02 %

IV. Residual Solvents

Method: ¹H-NMR

Result: 2.90 % Chloroform

V. Final Result

Total impurities (HPLC)	1.71 %
Water content	0.30 %
Residual solvents	2.90 %
Assay (100 % method) ¹	95.14 %

The assay is assessed to be 95.1 % 'as is'

The assay 'as is' is equivalent to the assay based on the not anhydrous and not dried substance respectively.

¹ The calculation of the 100 % method follows the formula:

$$\text{Assay (\%)} = (100 \% - \text{KF} - \text{RES}) \times \frac{\text{Purity HPLC (\%)}}{100 \%}$$

Water (KF) and Residual solvents (RES) are considered as absolute contributions, HPLC purity is considered as relative contribution.

LGCFOR1360.10 Lot Number 17217

LGC GmbH, Im Biotechnologiepark, TGZ II, D-14943 Luckenwalde, Germany