LoGiCal®
produced by LGC

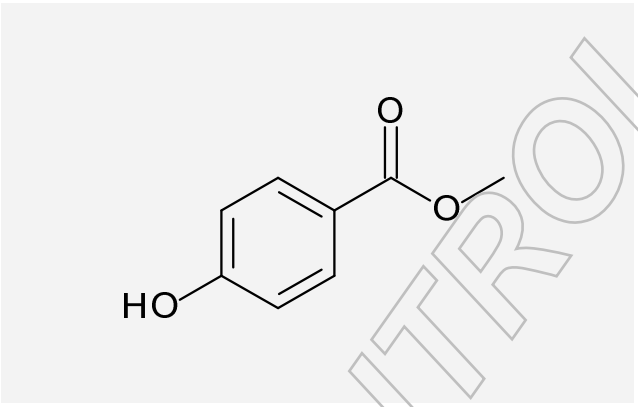
Certificate of Analysis

Reference Substance

Methyl Parahydroxybenzoate

Catalogue Number:	LGCFOR0431.00
Lot Number:	55747
Molecular Formula:	$C_8H_8O_3$
Molecular Weight:	152.15
CAS Number:	[99-76-3]

Long-term Storage:	2 to 8 °C, dark
Appearance:	white solid
Melting Point:	127 °C
Assay 'as is':	100 %



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: 2014-08-25

LGC GmbH

Dr. Sabine Schröder
Product Release

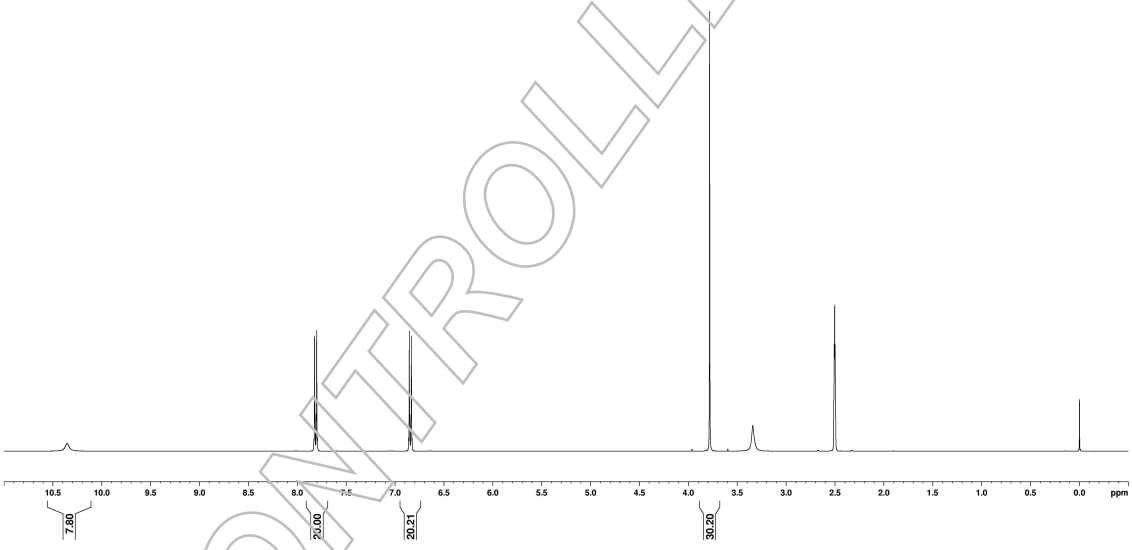
I. Identity

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

Ia. ^{1}H-NMR Spectrum

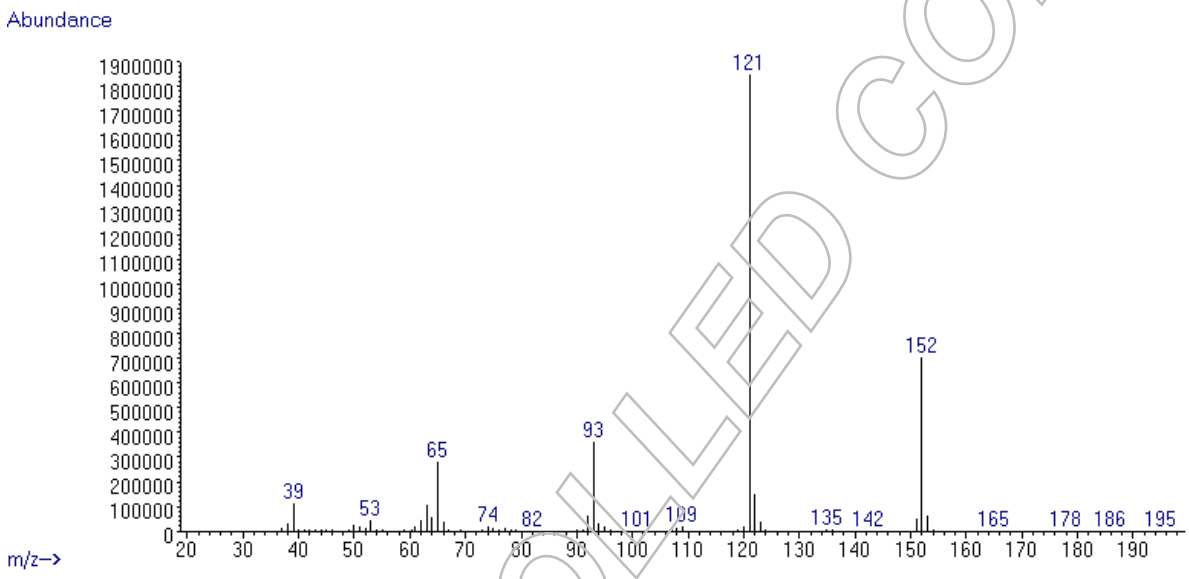
Conditions: 400 MHz, DMSO-d_6

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



Ib. Mass Spectrum

Method: EI, 70eV, detector temperature: 280 °C

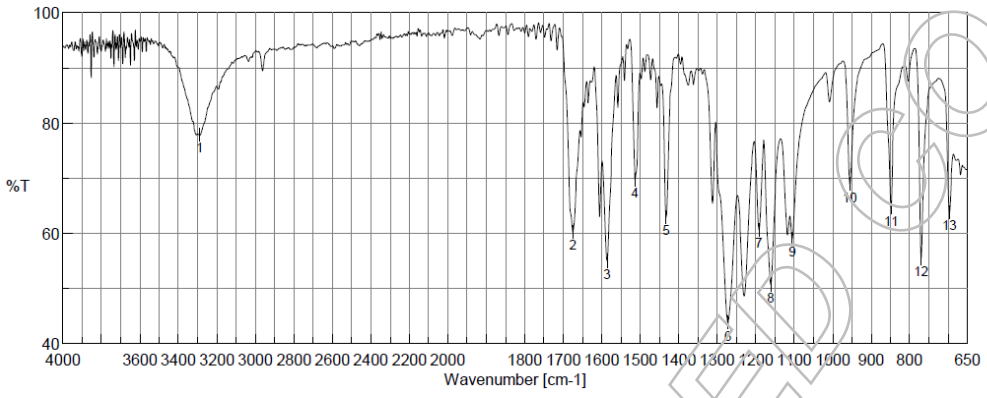


m/z	fragments
152	[M]
121	[M – CH_3O]
93	[M – $C_2H_3O_2$]

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



Result of Peak Picking

No.	Position	Intensity
1	3288.04	77.8227
2	1674.87	60.2468
3	1586.16	54.9865
4	1512.88	69.7179
5	1432.85	62.8758
6	1272.79	43.8048
7	1191.79	60.6422
8	1160.94	50.7096
9	1105.01	59.0415
10	955.555	68.9586
11	848.525	64.6208
12	770.423	55.5028
13	697.141	63.8149

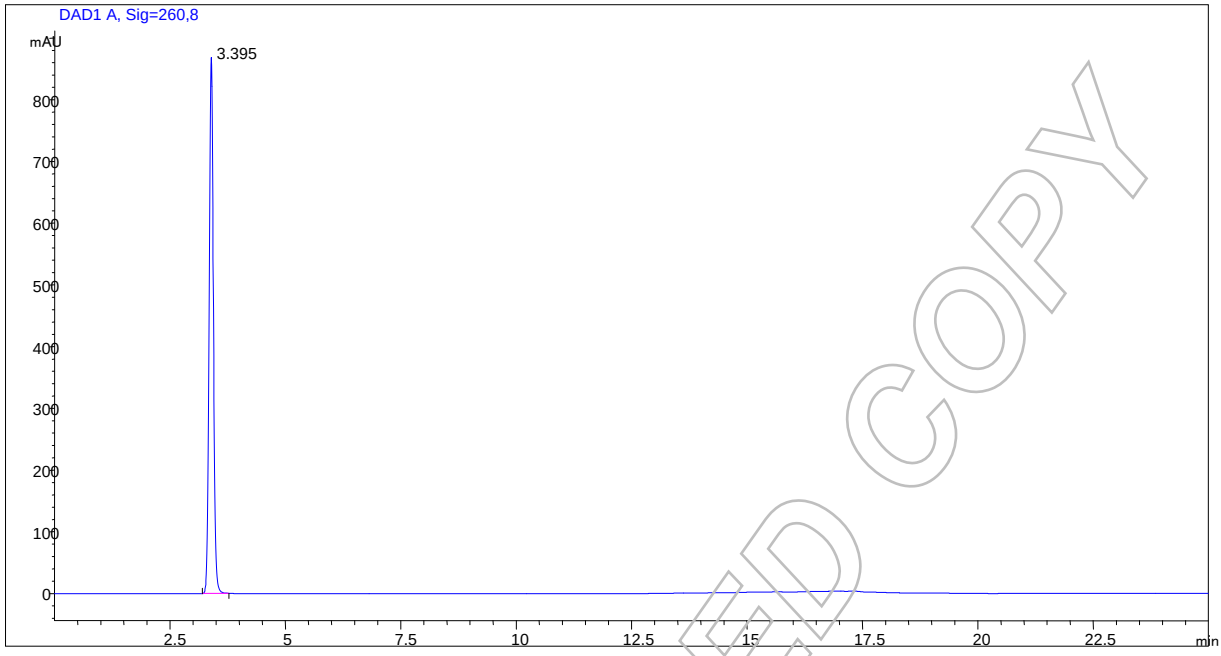
The signals of the IR spectrum and their interpretation are consistent with the structural formula.

II. Purity

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

HPLC Conditions:

Column:	**Conditions:**	**Detector:**	**Injector:**
RP 60 Select B 5 µm, 125 x 4 mm	1.0 ml/min, 40 °C 0-10 min Water/Acetonitrile 70/30 10-15 min Water/Acetonitrile to 30/70 15-20 min Water/Acetonitrile to 70/30 20-25 min Water/Acetonitrile 70/30 (v/v); 0.1 % H_3PO_4	DAD 260 nm	Auto 3 µl; 0.05734 mg/ml in Water/Acetonitrile 75/25 (v/v)



Area Percent Report - Sorted by Signal

Pk #	Retention Time	Area	Area %
1	3.39	5509.75	100.00
Totals		5509.75	100.00

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

Results:

Average	100 %
Number of results	n=6
Standard deviation	< 0.01 %

III. Water Content

Method: Karl Fischer titration

No significant amounts of water were detected (< 0.05 %).

IV. Residual Solvents

Method: ^{1}H-NMR

No significant amounts of residual solvents were detected (< 0.05 %)

V. Final Result

Total impurities (HPLC)	0.00 %
Water content	No significant amounts of water were detected (< 0.05 %).
Residual solvents	No significant amounts of residual solvents were detected (< 0.05 %)
Assay (100 % method)[1]	100.00 %

The assay is assessed to be 100 % ‘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:

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

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