

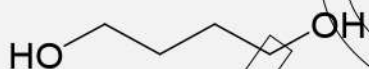
Certificate of Analysis

Reference Substance

1,4-Butanediol

Catalogue Number: LGCFOR1275.52
 Lot Number: 18969
 Molecular Formula: C₄H₁₀O₂
 Molecular Weight: 90.12
 CAS Number: [110-63-4]

Long-term Storage: 2 to 8 °C, dark
 Appearance: colourless viscous liquid
 very hygroscopic
 Assay 'as is': 99.7 %



Date of shipment: **2020-November-30**

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

Release Date: 2012-09-28

LGC GmbH



Dr. Sabine Schröder
Product Release

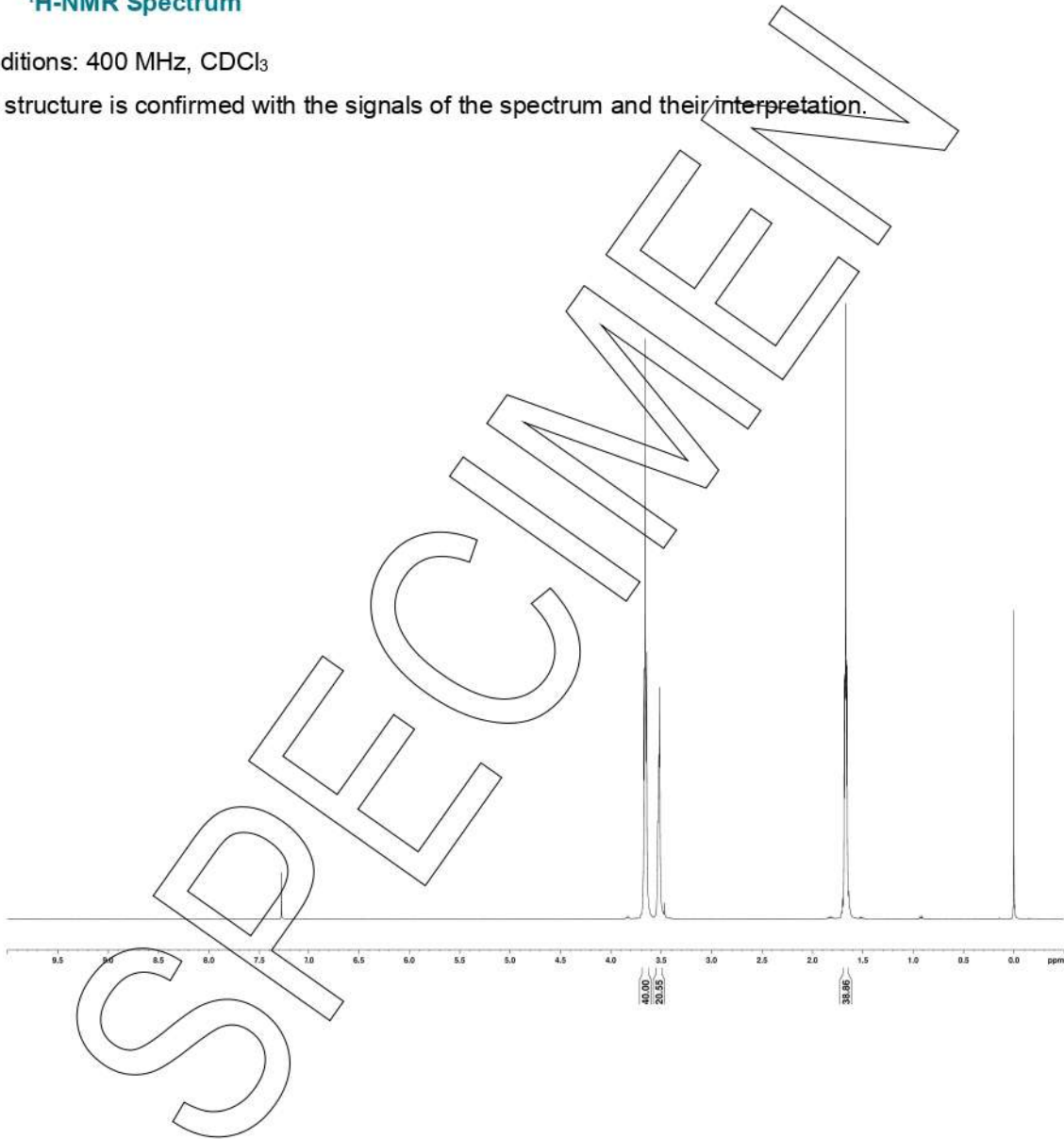
I. Identity

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

Ia. ¹H-NMR Spectrum

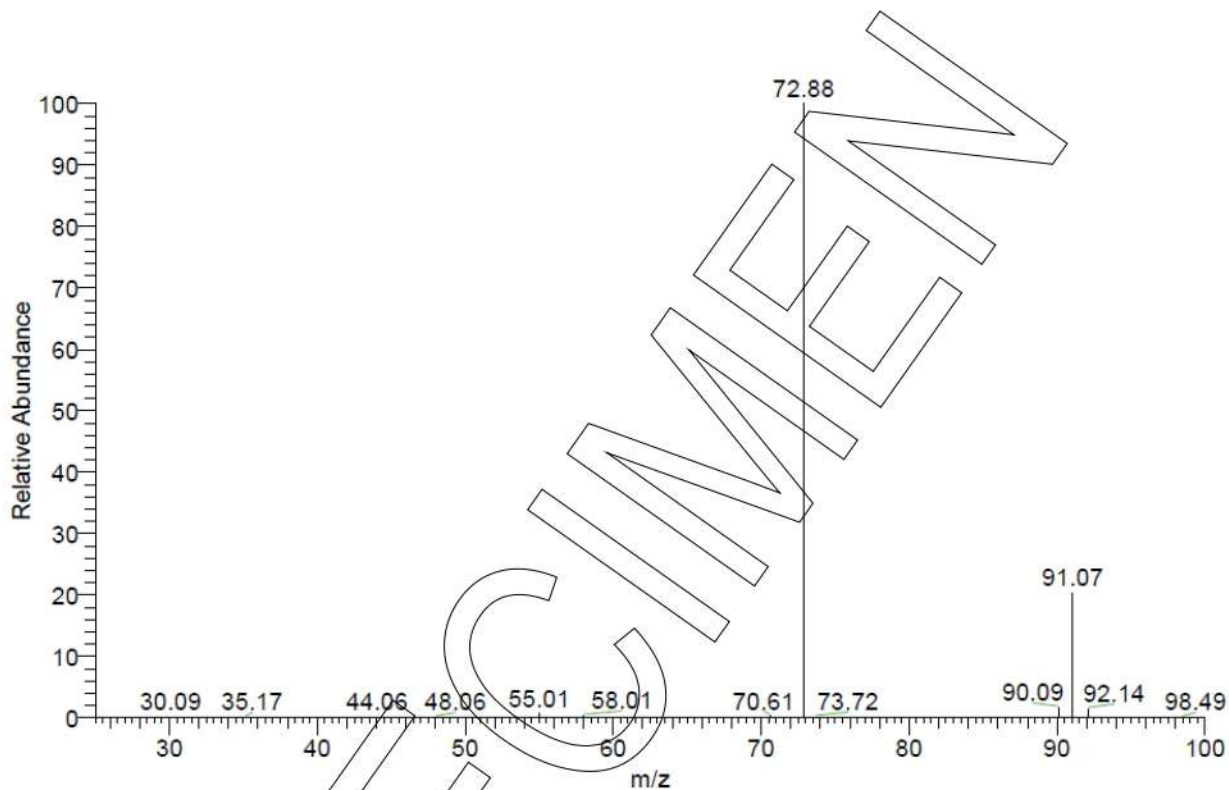
Conditions: 400 MHz, CDCl₃

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



Ib. Mass Spectrum

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



m/z	fragments
91	[MH]
73	[MH - H ₂ O]

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 gas chromatography (GC).

GC Conditions:

Column:

HP-5MS
30 m x 0.25 mm x 0.25 μ m

Injector and Flow:

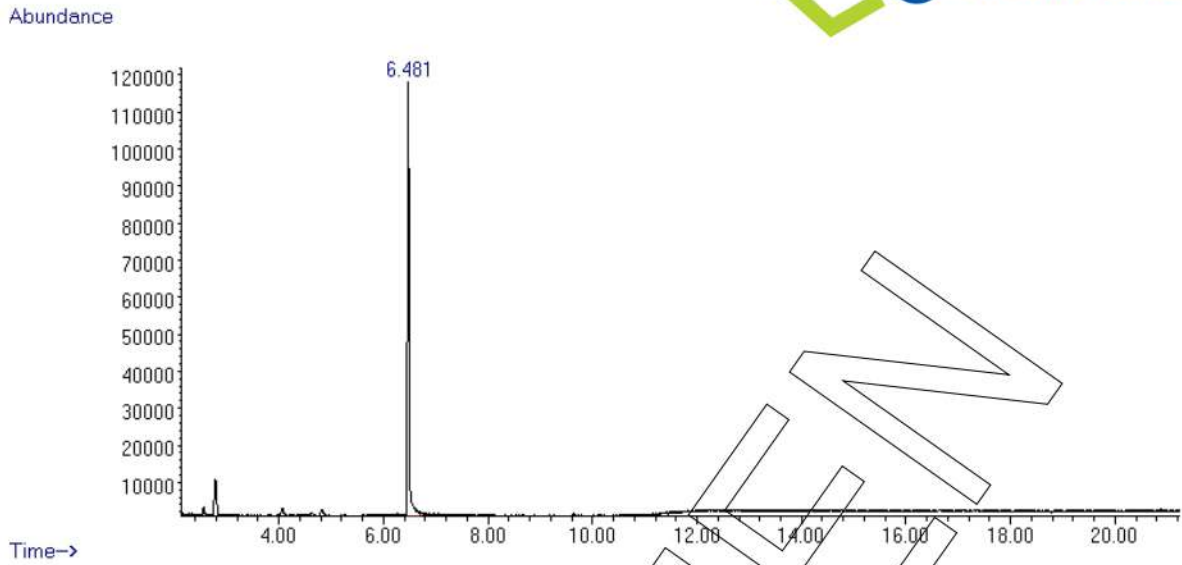
Split 20:1, 220 °C
Helium 1.50 ml/min

Oven Program:

Initial Temp.: 50 °C for 5 min
Heating Rate: 40 °C/min
Final Temp.: 300 °C for 10 min

Detector:

EI, 70 eV
35 to 550 amu
280 °C



Area Percent Report - Sorted by Signal

Pk #	Retention Time	Area	Area %
1	6.481	2675593	100.00
Totals		2675593	100.00

For the calculation the air 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 100 %
 Number of results n=3
 Standard deviation < 0.01 %

III. Water Content

Method: Karl Fischer titration

Results:

Average 0.19 %
 Number of results n=3
 Standard deviation 0.01 %

IV. Residual Solvents

Method: ¹H-NMR

Result: 0.15 % Methanol

V. Final Result

Total impurities (GC)	0.00 %
Water content	0.19 %
Residual solvents	0.15 %
Assay (100 % method)¹	99.66 %

The assay is assessed to be 99.7 % 'as is'

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

SPECIMEN

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

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