LoGiCal®
produced by LGC

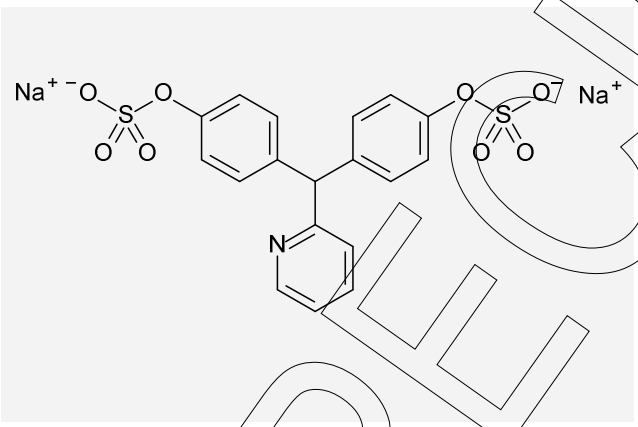
Certificate of Analysis

Reference Substance

Sodium Picosulfate

Catalogue Number:	LGCFOR0054.00
Lot Number:	51235
Molecular Formula:	$C_{18}H_{13}NNa_2O_8S_2$
Molecular Weight:	481.41
CAS Number:	[10040-45-6]

Long-term Storage:	2 to 8 °C, dark
Appearance:	white solid
Melting Point:	264 °C (dec.)
Assay 'as is':	95.6 %



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: 2014-06-20

LGC GmbH

Dr. Sabine Schröder
Product Release

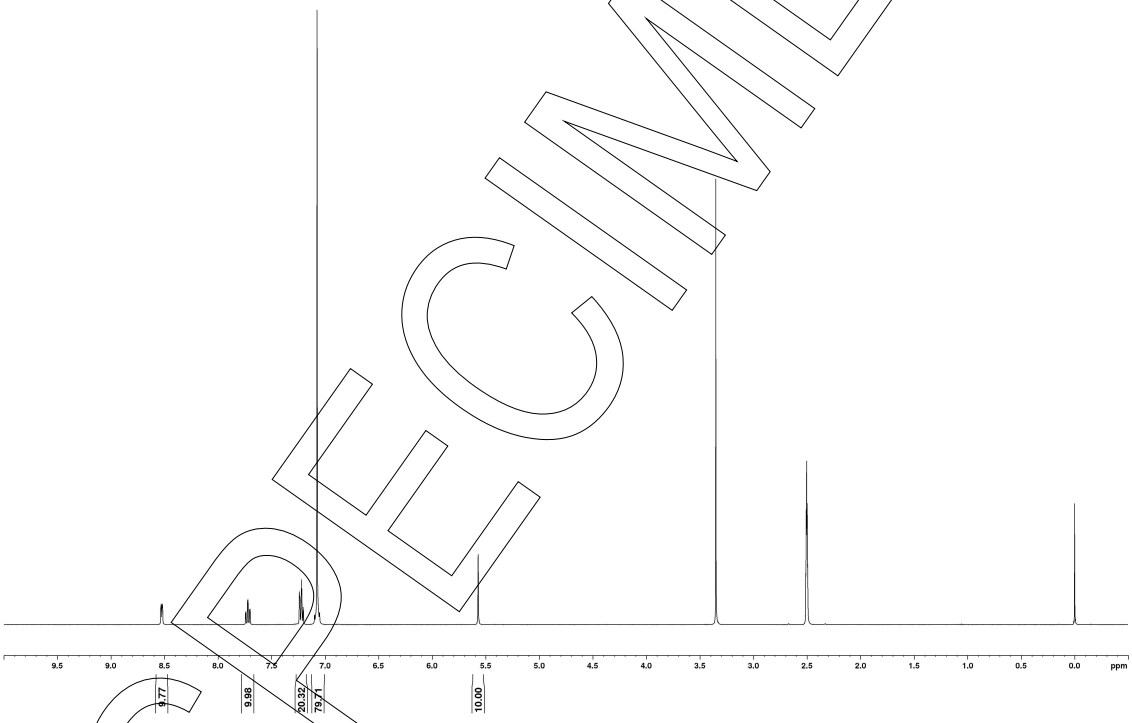
I. Identity

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

Ia. ^{1}H-NMR Spectrum

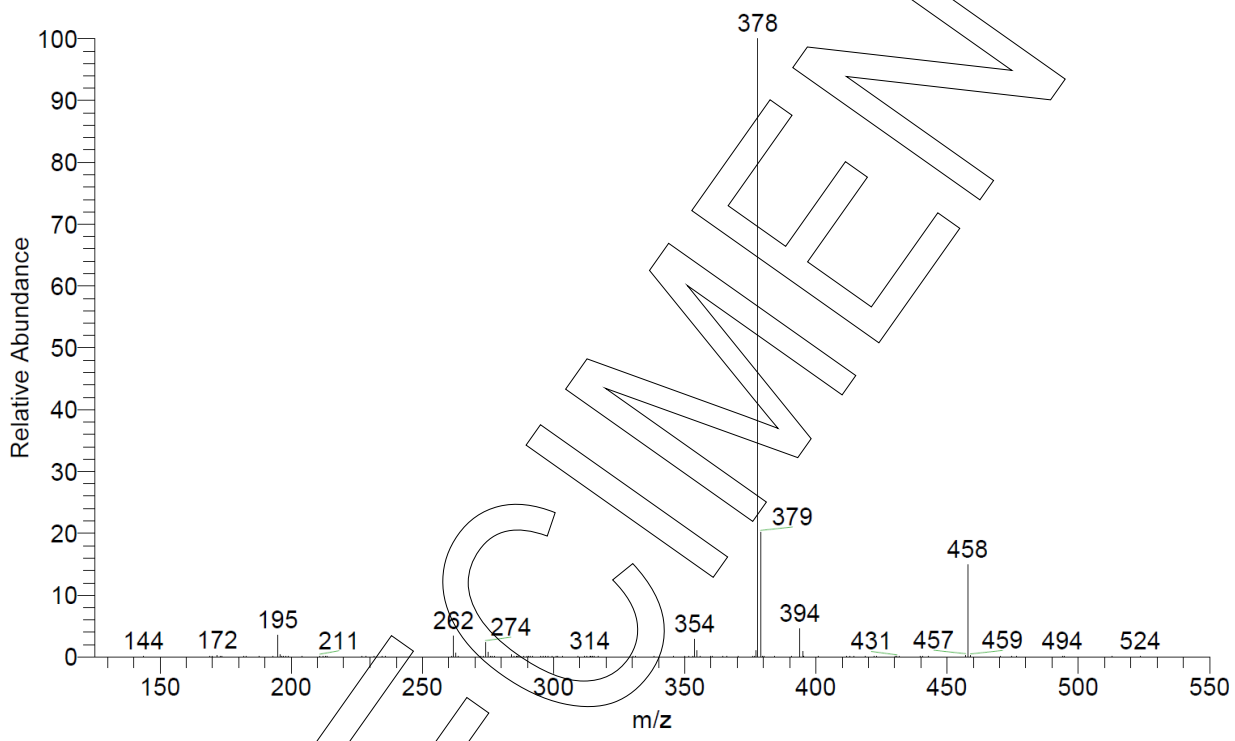
Conditions: 400 MHz, DMSO-d_6

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



Ib. Mass Spectrum

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

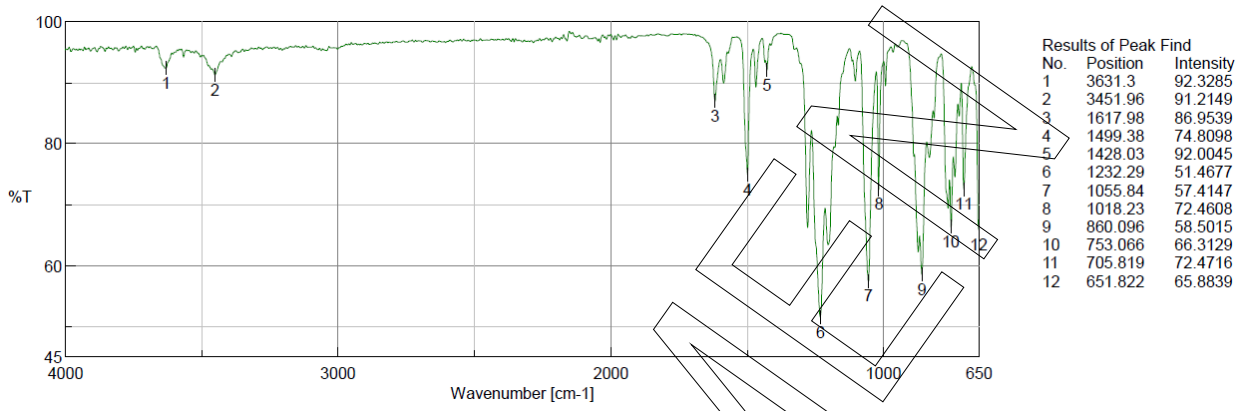


m/z	fragments
458	[M – Na]
378	[458 – SO_3]

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



Results of Peak Find

No.	Position	Intensity
1	3631.3	92.3285
2	3451.96	91.2149
3	1617.98	86.9539
4	1499.38	74.8098
5	1428.03	92.0045
6	1232.29	51.4677
7	1055.84	57.4147
8	1018.23	72.4608
9	860.096	58.5015
10	753.066	66.3129
11	705.819	72.4716
12	651.822	65.8839

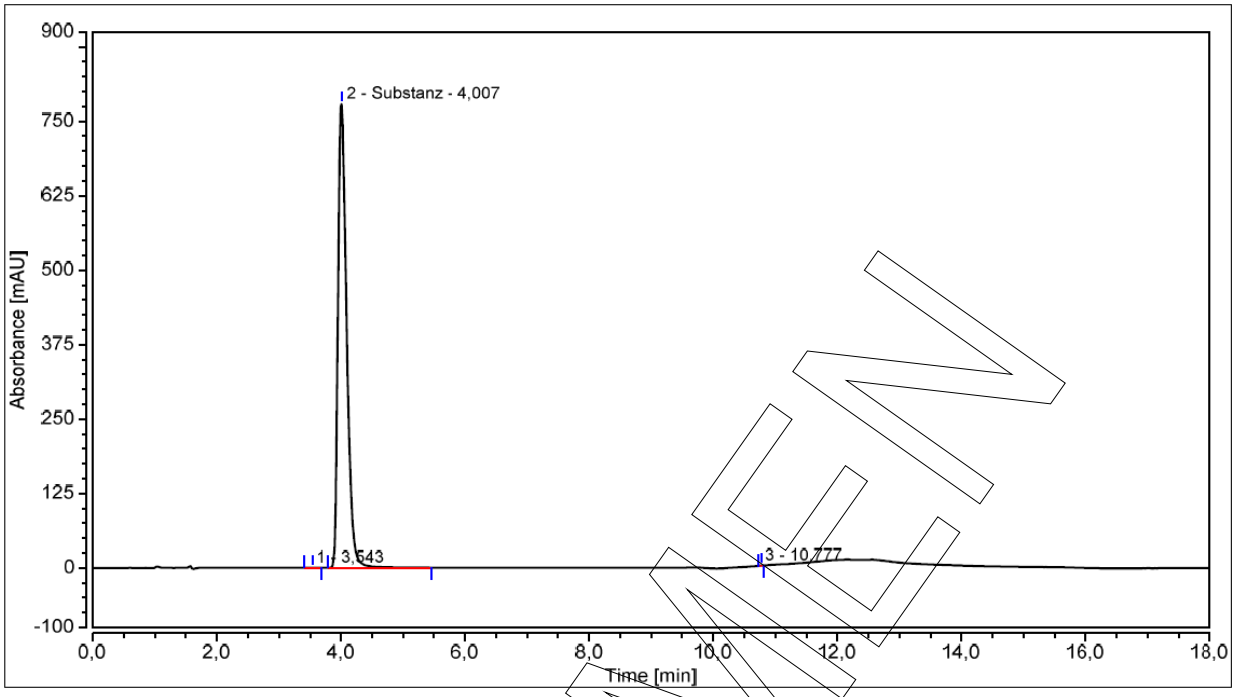
The signals of the IR spectrum and their interpretation are consistent with the structural formula.

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 0-7 min Water/Acetonitrile 95/5 7-10 min Water/Acetonitrile to 50/50 10-13 min Water/Acetonitrile to 95/5 13-18 min Water/Acetonitrile 95/5 (v/v); 0.1 % H_3PO_4	DAD 220 nm	Auto 10 µl; 0.062 mg/ml in Water



Area Percent Report - Sorted by Signal

Pk #	Retention Time	Area	Area %
1	3.543	0.046	0.04
2	4.007	126.692	99.95
3	10.777	0.023	0.02
Totals		126.760	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	99.95 %
Number of results	n=3
Standard deviation	< 0.01 %

III. Water Content

Method: Karl Fischer titration

Results:

Average	4.40 %
Number of results	n=3
Standard deviation	0.07 %

IV. Residual Solvents

Method: ^{1}H-NMR

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

V. Final Result

Total impurities (HPLC)	0.05 %
Water content	4.40 %
Residual solvents	No significant amounts of residual solvents were detected (< 0.05 %).
Assay (100 % method)[1]	95.55 %

The assay is assessed to be 95.6 % ‘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.