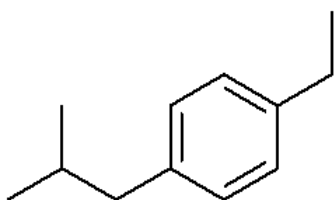




# Certificate of Analysis

## Reference Standard

1-Ethyl-4-isobutylbenzene



Molecular Formula: C<sub>12</sub>H<sub>18</sub>  
Molecular Weight: 162.27  
CAS Number: 100319-40-2

Catalogue Number: MM0002.25  
Lot Number: 451884  
Long-term Storage: 2 to 8 °C, dark  
Appearance: colourless liquid  
Assay 'as is': 98.6 %

Date of shipment: **2018-October-29**

This certificate is valid two years from the date of shipment provided the substance is stored under the recommended conditions unopened in the original container.

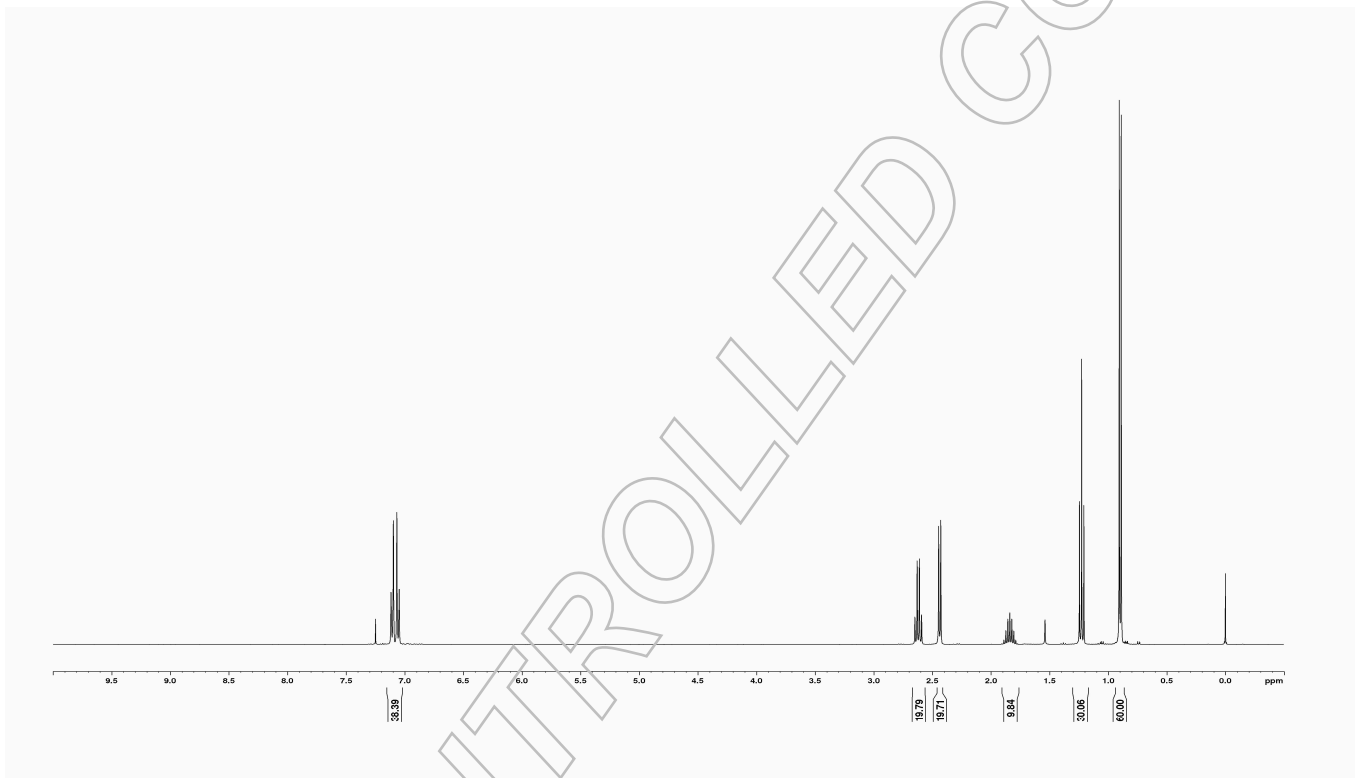


## I. Identity

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

### 1a. <sup>1</sup>H-NMR Spectrum

Conditions: 400 MHz, CDCl<sub>3</sub>

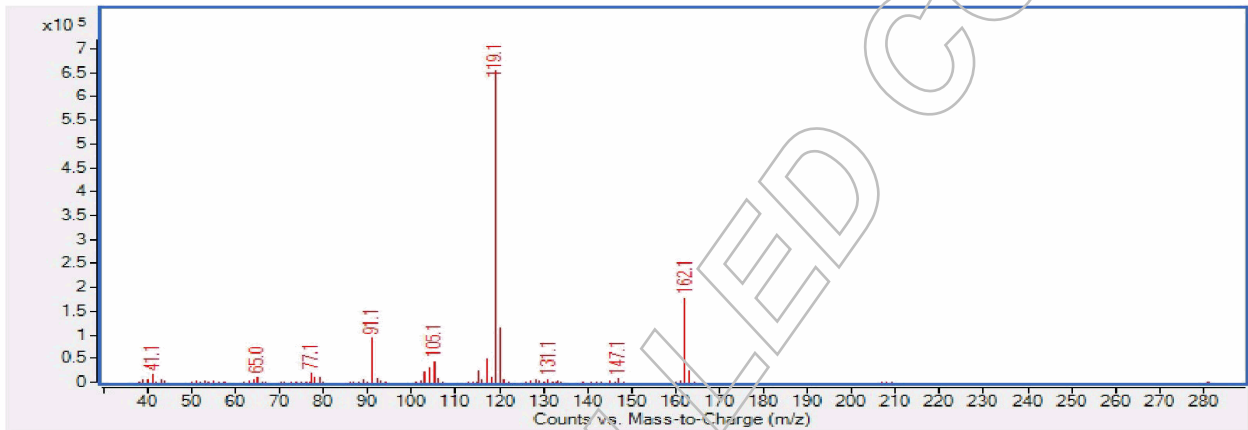


The structure is confirmed by the signals of the spectrum and their interpretation.



## Ib. Mass Spectrum

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

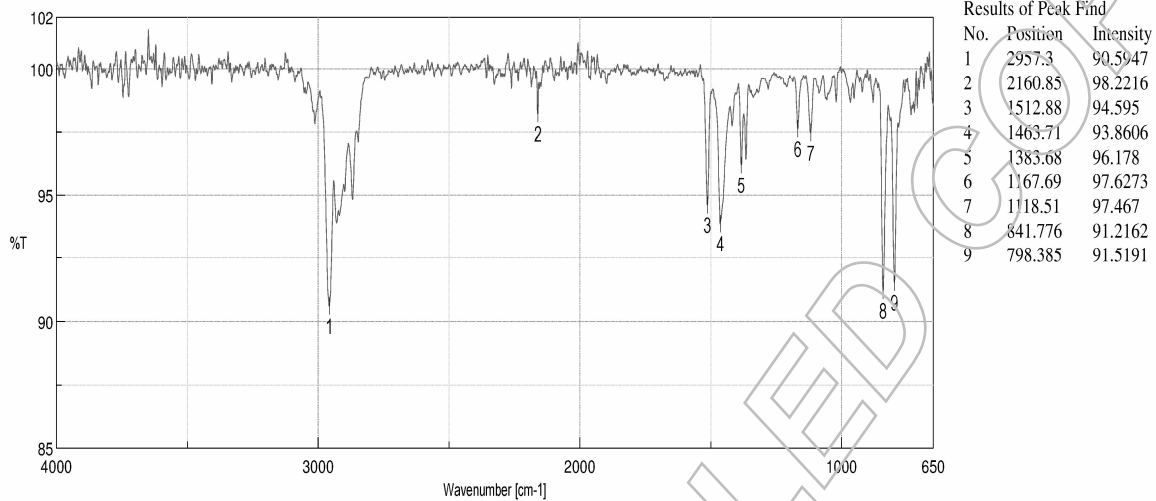


The signals of the MS spectrum and their interpretation are consistent with the structural formula.



## 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 structural formula.



## II. Purity

### IIa. Gas chromatography (GC)

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 µm

**Injector and Flow:**

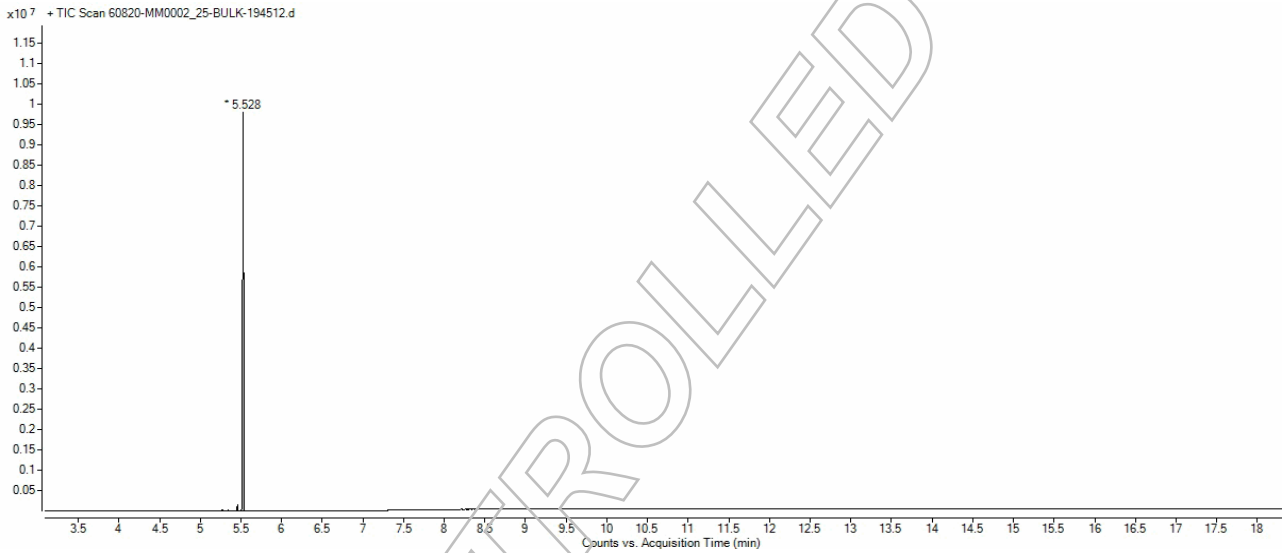
Split 20:1, 220 °C  
Helium 1.50 ml/min

**Oven Program:**

Initial Temp.: 70 °C for 3 min  
Heating Rate: 30 °C/min  
Final Temp.: 250 °C for 11 min

**Detector:**

EI, 70 eV  
35 to 550 amu  
280 °C



#### Area Percent Report - Sorted by Signal

Pk#	Retention Time	Area	Area %
1	5.269	29524.75	0.35
2	5.346	9701.79	0.12
3	5.458	102365.62	1.23
4	5.499	5325.55	0.06
5	5.528	8196714.17	98.14
6	5.775	6079.37	0.07
7	5.946	2534.01	0.03
Totals		<b>8352245.2600</b>	<b>100.00</b>

For the calculation the air 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:**

<b>Average</b>	98.18 %
<b>Number of results</b>	n=3
<b>Standard deviation</b>	0.04 %

**IIb. Water Content**

Method: Karl Fischer titration

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

**IIc. Residual Solvents**

Method: <sup>1</sup>H-NMR

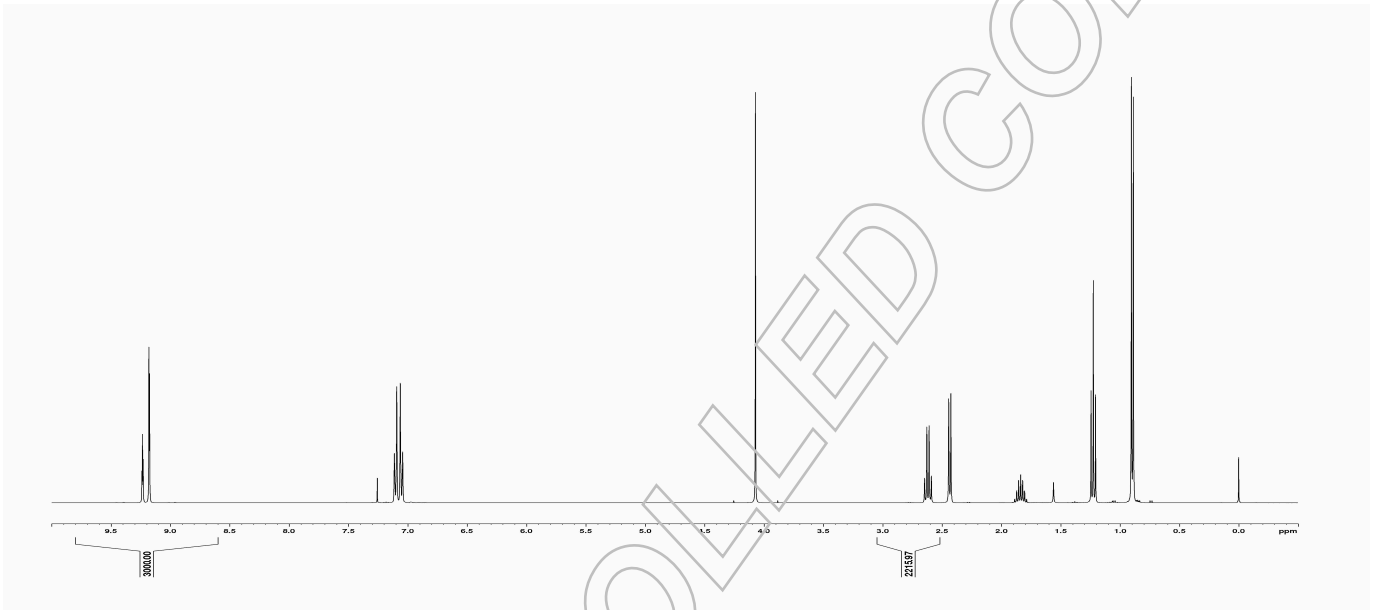
No significant amounts of residual solvents were detected (< 0.05 %).

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### III. Assay by quantitative NMR spectroscopy

The assay of the reference substance was established by quantitative NMR spectroscopy using  $\text{CDCl}_3$  as solvent and with Methyl 3,5-dinitrobenzoate (certified reference material, signal 8.6 - 9.8 ppm, 3 H) as internal standard.



**Results:**

<b>Average</b>	98.62 %
<b>Number of results</b>	n=6
<b>Standard deviation</b>	0.05 %



#### IV. Final Result

<b>Chromatographic purity (GC)</b>	98.18 %
<b>Water content</b>	No significant amounts of water were detected (< 0.05 %)
<b>Residual solvents</b>	No significant amounts of residual solvents were detected (< 0.05 %)
<b>Assay</b>	
<b>Quantitative NMR spectroscopy</b>	98.62 %

The assay is assessed to be 98.6 % 'as is'

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

Release Date:

Luckenwalde, 2018-July-31

Signed:

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Dr. Sabine Schröder  
Product Release