



# CERTIFICATE OF ANALYSIS

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## 1. Identification

**CAS Number:**

1416711-53-9

**Catalogue Number:**

TRC-B693603

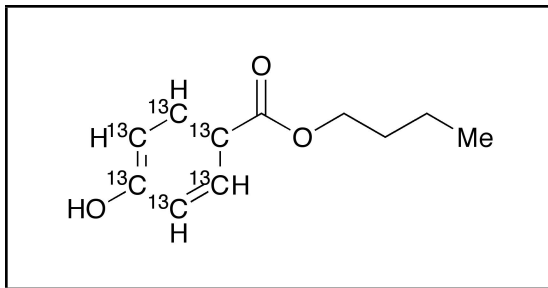
**Product:**

Butyl Paraben- $^{13}\text{C}_6$

**Synonyms:**

4-Hydroxybenzoic Acid- $^{13}\text{C}_6$  Butyl Ester; 4-(Butoxy-carbonyl)phenol- $^{13}\text{C}_6$ ; Aseptiform- $^{13}\text{C}_6$  Butyl; Butoben- $^{13}\text{C}_6$ ; Butyl 4-Hydroxybenzoate- $^{13}\text{C}_6$ ; Butyl Butex- $^{13}\text{C}_6$ ; Butyl Tegosept- $^{13}\text{C}_6$ ; Butyl Chemosept- $^{13}\text{C}_6$ ; n-Butylparaben- $^{13}\text{C}_6$ ; Preserval B- $^{13}\text{C}_6$ ; SPF- $^{13}\text{C}_6$ ; Solbrol B- $^{13}\text{C}_6$ .

**Structure:**



**Molecular Formula:**

$\text{C}_5^{13}\text{C}_6\text{H}_{14}\text{O}_3$

**Molecular Weight:**

200.18

**Source of Product:**

Synthetic

## 2. Analytical Information

**Lot Number:**

6-NKM-152-1

**Atmosphere:**

Air

**Melting Point:**

68 - 70°C

**Solubility**

Chloroform (Slightly), DMSO (Slightly), Methanol (Slightly)

**Appearance of Product:**

White to Off-White Solid

**Stability**

Not Determined

**Method for Determining Identity:**

$^1\text{H}$  NMR ( $\text{CDCl}_3$ ,  $\text{DMSO}-d_6$ ),  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ,  $\text{DMSO}-d_6$ ), and MS

**Long Term Storage Condition:**

4°C

**Purity:**

Chemical Purity: 98%

Isotopic Purity: 99.6%

99.97% by HPLC

**Shipping Condition**

This Product Is Stable To Be Shipped At Room Temperature

**Additional Information:**

TLC Conditions:  $\text{SiO}_2$ ; Dichloromethane : Methanol = 9 : 1; Visualized with UV and AMCS; Single Spot,  $R_f$  = 0.75.

$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, and MS conform to structure.

Elemental Analysis: (Found) %C: 66.14, %H: 6.97; (Calculated) %C: 65.96, %H: 7.05

Normalized Intensity:  $^{13}\text{C}_0$  = 0.01%,  $^{13}\text{C}_1$  = 0.04%,  $^{13}\text{C}_2$  = 0.02%,  $^{13}\text{C}_3$  = 0.01%,  $^{13}\text{C}_4$  = 0.03%  $^{13}\text{C}_5$  = 2.10%,  $^{13}\text{C}_6$  = 97.79%

Purity is based on the analytical results of the tests performed. NMR and Elemental Analysis (if available) may have an accuracy of  $\pm 2\%$ . Isotopic purity is based on mass distribution observed.

The contents of the specifications are subject to change without advance notice, and the specification values displayed here are the most up to date values.

Philip Chan, Head of Quality Assurance

**QC Test Date**

July 18, 2018

**Retest Date**

July 16, 2022