

CERTIFICATE OF ANALYSIS

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1. Identification

CAS Number: 362049-51-2

Catalogue Number: TRC-M325663

Product:

Methyl Paraben-d4

Synonyms:

4-Hydroxybenzoic Acid-d4 Methyl Ester; 4-Carbomethoxyphenol-d4; 4-Methoxycarbonylphenol-d4; 4-Hydroxymethylbenzoate-d4; Danisol M-d4; E 218-d4; Killitol-d4; Maseptol-d4; Mekkings M-d4; Metaben-d4; Metagin-d4; Preserval-d4; Solbrol-d4;

Structure:

Molecular Formula:

 $C_8H_4D_4O_3$

Molecular Weight:

156.17

Source of Product:

Synthetic

2. Analytical Information

Lot Number:

2-TIF-74-1

Melting Point:

123 - 125°C

Appearance of Product:

White to Off-White Solid

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Method for Determining Identity:

¹H NMR (DMSO-d₆) and MS

Purity:

Chemical Purity: 97% Isotopic Purity: 98.6%

Atmosphere:

Air

Solubility

DMSO (Slightly), Methanol (Slightly, Heated)

Stability

Not Determined

Long Term Storage Condition:

4°C

Shipping Condition

This Product Is Stable To Be Shipped At Room Temperature

Additional Information:

TLC Conditions: SiO₂; Dichloromethane: Methanol = 9:1; Visualized with UV and KMnO₄; Single Spot, Rf = 0.40.

¹H NMR and MS conform to structure.

Elemental Analysis: (Found) %C: 61.36, %H: 5.21; (Calculated) %C: 61.53, %H: 5.17

Normalized Intensity: $d_0 = 0.09\%$, $d_1 = 0.03\%$, $d_2 = 0.10\%$, $d_3 = 4.83\%$, $d_4 = 94.96\%$

Purity is based on the analytical results of the tests performed. NMR and Elemental Analysis (if available) may have an accuracy of ± 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
September 11, 2017

Retest Date
September 9, 2021