

02.16 p02 65

# CERTIFICATE OF ANALYSIS

## 1. Identification

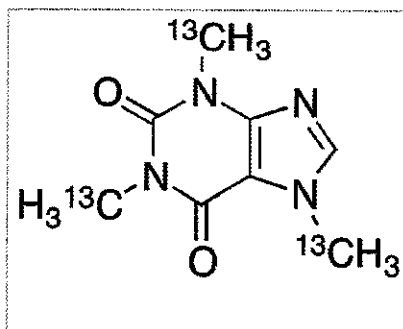
**Catalogue Number:** C080101

**CAS Number:** 78072-66-9

**Product:** Caffeine-13C3

**Synonym:** 3,7-Dihydro-1,3,7-tri(methyl-13C)-1H-purine-2,6-dione; 1,4,6-Trimethyl-1H-imidazo [4,5-b]pyridine-5,7(4H,6H)-dione-13C3; 1,3,7-Trimethylxanthine-13C3; 7-Methyltheophylline-13C3; Alert-Pep-13C3; Cafalgine-13C3; Cafeina-13C3; Caffedrine-13C3; Caffein-13C3; Cafipel-13C3; DHCplus-13C3; Dasin-13C3; Diurex-13C3; Durvitan-13C3; Guaranine-13C3; Hycomine-13C3; Koffein-13C3; Mateina-13C3; Methyltheobromine-13C3; Miudol-13C3; NSC 5036-13C3; New Cetamol-13C3; No-Doz-13C3; Palergot-C-13C3; Phensal-13C3; Refre

**Structure:**



**Molecular Formula:**

C<sub>5</sub><sup>13</sup>C<sub>3</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>

**Molecular weight:**

197.15

**Source of Product:**

N/A

**Solubility:**

DMSO (Slightly, Heated), Methanol (Slightly, Heated)

**Lot Number:** 1-AWT-26-1

**Purity:** Chemical Purity: 98.0% Isotopic Purity: 99.0%

**Shipping Condition:** This Product Is Stable To Be Shipped At Room Temperature

**Storage Condition:** Refrigerator

## 2. Warning

**Warning 1:**

**Warning 2:**

**Warning 3:**

## 3. Analytical Information

Tests:	Specifications:	Results:
NMR	Conforms to structure	Conforms
MS	Conforms to Structure	Conforms
Melting Point	Report Results	234 - 236°C
C NMR	Conforms to Structure	Conforms
Elemental Analysis	Conforms	Refer: Additional Information
Appearance		White Solid

### Additional Information:

TLC Conditions: SiO<sub>2</sub>; Dichloromethane : Methanol = 9 : 1; Visualized with UV and AMCS; Single Spot, R<sub>f</sub> = 0.55. 1H NMR, 13C NMR, and MS conform to structure. Elemental Analysis: (Found) %C: 48.83, %H: 5.00, %N: 28.22; (Calculated) %C: 48.71, %H: 5.11, %N: 28.42 Normalized Intensity: 13C0 = 0.10%, 13C1 = 0.03%, 13C2 = 2.71%, 13C3 = 97.16%

Purity is based on the analytical results of the tests performed. NMR and TLC may have an accuracy +-2%. Isotopic purity is based on mass distribution observed.

## 4. Signatures

<b>Reviewed By</b>	<b>Reviewed By</b>	<b>C of A Approved By</b>	<b>Test Date</b>	<b>Retest Date</b>
			10/24/2016	10/22/2020

Philip Chan

