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Certificate of Analysis

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Print Date: Oct 15th 2018

Product Name: CBM 301940

CAS Number: 902146-11-6

IUPAC Name: tert-Butyl 3-(5-(1,1,1,3,3,3-hexafluoro-2-hydroxypropan-2-yl)-4,5-dihydroisoxazole-3-carboxamido)butanoate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Weight: Physical Appearance: Solubility: 422.32 Off White solid DMSO to 100 mM ethanol to 100 mM Store at -20°C

Storage: **Batch Molecular Structure:**

CF₃

2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis: $R_{f} = 0.4 \text{ (Ethyl acetate:Petroleum ether [3:7])}$ Shows 99.4% purity
Consistent with structure
Consistent with structure
Carbon Hydrogen Nitrogen
Theoretical 42.66 4.77 6.63
Found 42.97 4.78 6.55

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Catalog No.: 6319 Batch No.: 1

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tert-Butyl 3-(5-(1,1,1,3,3,3-hexafluoro-2-hydroxypropan-2-yl)-4,5-dihydroisoxazole-3-carboxamido)butanoate

Description:

IUPAC Name:

Potent malonyl-CoA decarboxylase (MCD) inhibitor ($IC_{50} = 23$ nM). Suppresses malonyl-CoA degradation and fatty acid oxidation in isolated rat hearts, leading to secondary increase in glucose oxidation. Improves cardiac function during reperfusion of ischemic isolated rat hearts. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Weight: 422.32

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info: DMSO to 100 mM ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Catalog No.: 6319

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Cheng *et al* (2006) Discovery of potent and orally available malonyl-CoA decarboxylase inhibitors as cardioprotective agents. J.Med.Chem. **49** 4055. PMID: 16821767.

Dyck *et al* (2004) Malonyl coenzyme a decarboxylase inhibition protects the ischemic heart by inhibiting fatty acid oxidation and stimulating glucose oxidation. Circ.Res. **94** e78. PMID: 15105298.

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