

Certificate of Analysis

Print Date: Mar 23rd 2023

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Product Name: TC-S 7009 Catalog No.: 5243 Batch No.: 2

CAS Number: 1422955-31-4

IUPAC Name: N-(3-Chloro-5-fluorophenyl)-4-nitro-2,1,3-benzoxadiazol-5-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_6CIFN_4O_3$

Batch Molecular Weight: 308.65

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.38$ (Ethyl acetate:Petroleum ether [15:85])

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 46.7 1.96 18.14 Found 46.57 1.9 18.17



Product Information

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IUPAC Name: N-(3-Chloro-5-fluorophenyl)-4-nitro-2,1,3-benzoxadiazol-5-amine

Description:

TC-S 7009 is a high affinity and selective HIF-2 α inhibitor (K_d = 81 nM). Binds to the HIF-2 α PAS-B domain; disrupts HIF-2 α -ARNT heterodimerization. Exhibits >60-fold selectivity for HIF-2 α over HIF-1 α . Decreases HIF-2 α DNA-binding and attenuates expression of HIF-2 α target genes in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₂H₆CIFN₄O₃

Batch Molecular Weight: 308.65 Physical Appearance: Yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO 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).

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:

Wu et al (2019) Bidirectional modulation of HIF-2 activity through chemical ligands. Nat. Chem. Biol. 15 367. PMID: 30804532.

Rogers *et al* (2013) Development of inhibitors of the PAS-B domain of the HIF-2α transcription factor. J.Med.Chem. *56* 1739. PMID: 23363003.

Scheuermann *et al* (2013) Allosteric inhibition of hypoxia inducible factor-2 with small molecules. Nat.Chem.Biol. **9** 271. PMID: 23434853.

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