

Certificate of Analysis

Print Date: May 22nd 2020

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Product Name: NNC 0640 Catalog No.: 6807 Batch No.: 1

CAS Number: 307986-98-7

IUPAC Name: 4-[[(4-Cyclohexylphenyl)[[[3-(methylsulfonyl)phenyl]amino]carbonyl]amino]methyl]-N-2H-tetrazol-5-ylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{31}N_7O_4S.\frac{1}{4}H_2O$

Batch Molecular Weight: 578.17

Physical Appearance: White solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.24 5.49 16.96 Found 60.11 5.49 17.04

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Product Information

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IUPAC Name: 4-[[(4-Cyclohexylphenyl)[[[3-(methylsulfonyl)phenyl]amino]carbonyl]amino]methyl]-N-2H-tetrazol-5-ylbenzamide

Description:

Negative allosteric modulator of glucagon receptors (pK $_{\rm i}$ = 7.4). Binds to external surface of the transmembrane domain. Also negative allosteric modulator of glucagon-like peptide 1 (GLP-1) receptor. Inhibits GLP-1-mediated cAMP accumulation in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₉H₃₁N₇O₄S.1/4H₂O

Batch Molecular Weight: 578.17 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

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:

Song *et al* (2017) Human GLP-1 receptor transmembrane domain structure in complex with allosteric modulators. Nature. *546* 213. PMID: 28514449.

Zhang et al (2017) Structure of the full-length glucagon class B g-protein-coupled receptor. Nature. 546 259. PMID: 28514451.

Jazayeri et al (2016) Extra-helical binding site of a glucagon receptor antagonist. Nature. 533 274. PMID: 27111510.