

Certificate of Analysis

Print Date: May 6th 2021

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Product Name: AR-C 141990 hydrochloride Catalog No.: 5658 Batch No.: 2

CAS Number: 2250019-94-2

IUPAC Name: 5-[[(3R)-3-Hydroxy-1-pyrrolidinyl]-a-methyl-1-(2-methylpropyl)-6-(4-quinolinylmethyl)thieno[2,3-d]

pyrimidine-2,4(1H,3H)-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₈N₄O₄S.HCl.H₂O

Batch Molecular Weight: 547.07

Physical Appearance: Yellow solid

Solubility: water to 100 mM

DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

HCI

2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

¹³C NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.08 5.71 10.24 Found 56.91 5.73 10.15

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



Product Information

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Batch No.: 2

Product Name: AR-C 141990 hydrochloride

CAS Number: 2250019-94-2

IUPAC Name: 5-[[(3R)-3-Hydroxy-1-pyrrolidinyl]carbonyl]-3-methyl-1-(2-methylpropyl)-6-(4-quinolinylmethyl)thieno[2,3-d]

pyrimidine-2,4(1H,3H)-dione

Description:

Monocarboxylate transporter (MCT1) inhibitor (pK $_i$ = 7.6. Exhibits approximately 10-fold selectivity for MCT1 over MCT2 and no significant activity against MCT3 or 4. Inhibits graft versus host response and prolongs cardiac graft survival in a rat model. Immunosuppressant. Also inhibits brain penetration of GHB analog HOCPCA.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₆H₂₈N₄O₄S.HCl.H₂O

Batch Molecular Weight: 547.07 Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:

HCI

Storage: Store at -20°C. This product is packaged under an inert atmosphere.

Catalog No.: 5658

Solubility & Usage Info:

water to 100 mM DMSO to 100 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Thiesen et al (2015) In vitro and in vivo evidence for active brain uptake of the GHB analog HOCPCA by the monocarboxylate transporter subtype 1. J.Pharmacol.Exp.Ther. **354** 166. PMID: 25986445.

Påhlman *et al* (2012) Immunosuppressive properties of a series of novel inhibitors of the monocarboxylate transporter MCT-1. Transpl.Int. **26** 22. PMID: 23137339.

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