Certificate of Analysis

Print Date: Oct 7th 2019

Product Name: PHA 543613 hydrochloride

1586767-92-1

IUPAC Name: N-(3R)-1-Azabicyclo[2.2.2]oct-3-yl-furo[2,3-c]pyridine-5-carboxamide hydrochloride

312.28

Found

C₁₅H₁₇N₃O₂.HCI.¹/₄H₂O

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

TOCR

a biotechne

CAS Number:

White solid water to 100 mM DMSO to 25 mM Store at +4°C

Storage: **Batch Molecular Structure:**

.HCI

57.61

5.87

13.44

2. ANALYTICAL DATA

 HPLC:
 Shows 99.7% purity

 ¹H NMR:
 Consistent with structure

 Mass Spectrum:
 Consistent with structure

 Microanalysis:
 Carbon Hydrogen Nitrogen

 Theoretical 57.69
 5.97
 13.46

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

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www.tocris.com

Catalog No.: 3092

Batch No.: 4

C'R biotechne

Product Information

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Print Date: Oct 7th 2019

Product Name: PHA 543613 hydrochloride

CAS Number: 1586767-92-1

N-(3R)-1-Azabicyclo[2.2.2]oct-3-yl-furo[2,3-c]pyridine-5-carboxamide hydrochloride **IUPAC Name:**

Description:

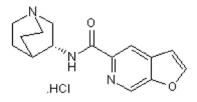
Potent α 7 nAChR agonist that displays selectivity over α 3 β 4, $\alpha 1\beta 1\gamma \delta$, $\alpha 4\beta 2$ and 5-HT₃ receptors. Positively influences sensory gating and memory in in vivo models of schizophrenia. Orally active and brain penetrant.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₅H₁₇N₃O₂.HCl.¹/₄H₂O Batch Molecular Weight: 312.28 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info: water to 100 mM DMSO to 25 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Acker et al (2008) Discovery of N-[3R,5R)-1-azabicyclo[3.2.1]ocy-3-yl]furo-[2,3-c]pyridine-5-carboxamide as an agonist of the α 7 nicotinic acetylcholine receptor: in vitro and in vivo activity. Bioorg.Med.Chem.Letts. 18 3611.

Faghih et al (2008) Allosteric modulators of the α7 nicotinic acetylcholine receptor. J.Med.Chem. 51 701. PMID: 18198823.

Wishka et al (2006) Discovery of N-[(3R)-1-azabicyclo[2.2.2]oct-3-yl]furo[2,3-c]pyridine-5-carboxamide, an agonist of the α7 nicotinic acetylcholine receptor, for the potential treatment of cognitive deficits in schizophrenia; synthesis and st J.Med.Chem. 49 4425. PMID: 16821801.

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