Print Date: Jan 21st 2019

Certificate of Analysis

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Product Name: **PHA 543613 hydrochloride** **Catalog No.: 3092** **Batch No.: 3**

CAS Number: 1586767-92-1

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{17}N_3O_2.2HCl.¼H_2O$

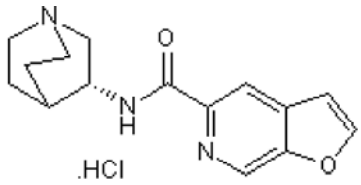
Batch Molecular Weight: 312.28

Physical Appearance: Off-white solid

Solubility: water to 100 mM
DMSO to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.69	5.97	13.46
Found	57.75	5.73	13.59

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

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Description:

Potent α7 nAChR agonist that displays selectivity over α3β4, α1β1γδ, α4β2 and 5-HT_3 receptors. Positively influences sensory gating and memory in in vivo models of schizophrenia. Orally active and brain penetrant.

Physical and Chemical Properties:

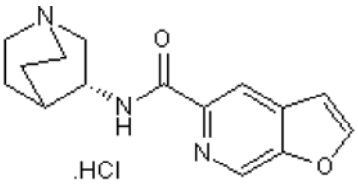
Batch Molecular Formula: $C_{15}H_{17}N_3O_2.2HCl.¼H_2O$

Batch Molecular Weight: 312.28

Physical Appearance: Off-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*-[3*R*,5*R*)-1-azabicyclo[3.2.1]ocy-3-yl]furo-[2,3-*c*]pyridine-5-carboxamide as an agonist of the α7 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*-[(3*R*)-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 structure-activity relationship. J.Med.Chem. ***49*** 4425. PMID: 16821801.

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