Print Date: Dec 12th 2017

# Certificate of Analysis

www.tocris.com

**Product Name:** **5-Iodo-A-85380 dihydrochloride** **Catalog No.: 1518** **Batch No.: 5**

CAS Number: 1217837-17-6

IUPAC Name: 3-[(2*S*)-2-Azetidinylmethoxy]-5-iodopyridine dihydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_9H_{11}IN_2O.2HCl.H_2O$

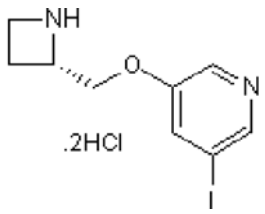
**Batch Molecular Weight:** 381.05

**Physical Appearance:** White solid

**Solubility:** water to 100 mM
DMSO to 100 mM

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**HPLC:** Shows 99.8% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** $[\alpha]_D$ = -7.8 (Concentration = 1, Solvent = Water)

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 28.37 | 3.97 | 7.35 |
| Found | 28.11 | 3.89 | 7.41 |



**bio-techne.com**
info@bio-techne.com
techsupport@bio-techne.com

**North America**
Tel: (800) 343 7475

**China**
info.cn@bio-techne.com
Tel: +86 (21) 52380373

**Europe Middle East Africa**
Tel: +44 (0)1235 529449

**Rest of World**
www.tocris.com/distributors
Tel:+1 612 379 2956

**Product Name:** **5-Iodo-A-85380 dihydrochloride** **Catalog No.: 1518** **Batch No.: 5**

CAS Number: 1217837-17-6

IUPAC Name: 3-[(2*S*)-2-Azetidinylmethoxy]-5-iodopyridine dihydrochloride

**Description:**

A highly potent and subtype-selective agonist for the α4β2 and α6β2 nicotinic acetylcholine receptors. Activates α-CTx-MII-sensitive and -insensitive components of [$^3$H]dopamine release from rat striatal synaptosomes, corresponding to α6β2 and α4β2 ($EC_{50}$ values are 12.7 and ~35 nM respectively). ~5000- , 25000- and 140000-fold selective over α3β4, α7 and muscle nAChR receptors respectively. Precursor also available.

**Physical and Chemical Properties:**

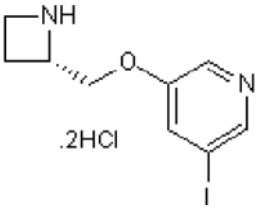
Batch Molecular Formula: $C_9H_{11}IN_2O.2HCl.H_2O$

Batch Molecular Weight: 381.05

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**




**Storage:** Desiccate at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

water to 100 mM
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:**

**Mogg** *et al* (2004) Functional responses and subunit composition of presynaptic nicotinic receptor subtypes explored using the novel agonist 5-iodo-A-85380. Neuropharmacology ***47*** 848. PMID: 15527819.

**Mukhin** *et al* (2000) 5-Iodo-A-85380, an α4β2 subtype-selective ligand for nicotinic acetylcholine receptors. Mol.Pharmacol. ***57*** 642. PMID: 10692507.

**Koren** *et al* (1998) 2-, 5-, and 6-Halo-3-(2(*S*)-azetidinylmethoxy)pyridines: synthesis, affinity for nicotinic acetylcholine receptors, and molecular modeling. J.Med.Chem. ***41*** 3690. PMID: 9733494.