

Product Name: AZD 2066

Catalog No.: 5614

Batch No.: 1

CAS Number: 934282-55-0

IUPAC Name: 4-[5-[(1*R*)-1-[5-(3-Chlorophenyl)-3-isoxazolyl]ethoxy]-4-methyl-4*H*-1,2,4-triazol-3-yl]pyridine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₆ClN₅O₂·¼H₂O

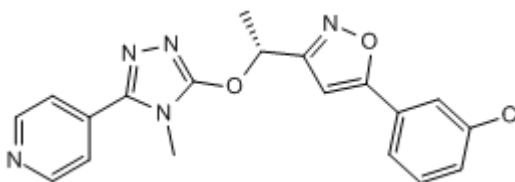
Batch Molecular Weight: 386.32

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -48.2 (Concentration = 5.8, Solvent = Chloroform)

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 59.07 4.3 18.13

Found 59.22 4.17 18.09

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

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Description:

mGlu₅ antagonist. Displays discriminative effects in rats. Orally bioavailable and brain penetrant.

Physical and Chemical Properties:

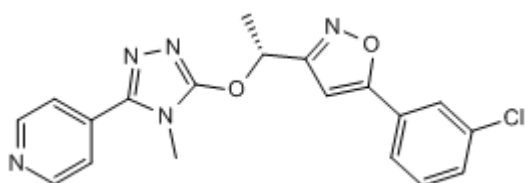
Batch Molecular Formula: C₁₉H₁₆ClN₅O₂ · ¼H₂O

Batch Molecular Weight: 386.32

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Swedberg et al (2014) AZD9272 and AZD2066: selective and highly central nervous system penetrant mGluR₅ antagonists characterized by their discriminative effects. *J.Pharmacol.Exp.Ther.* **350** 212. PMID: 24876235.

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