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Certificate of Analysis

www.tocris.com

Print Date: Mar 11th 2022

Product Name: (±)-5'-Chloro-5'-deoxy-ENBA

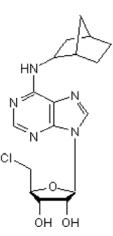
Catalog No.: 3576 Batch No.: 2

CAS Number: 103626-26-2 IUPAC Name: *N*-Bicyclo[2.2.1]hept-2-yl-5'-chloro-5'-deoxyadenosine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: $C_{17}H_{22}CIN_5O_3.1/4H_2O$ 384.34 White solid DMSO to 100 mM ethanol to 100 mM Store at -20°C

Storage: Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis: R_f = 0.32 (Dichloromethane:Methanol [9:1]) Shows >99.3% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 53.13 5.9 18.22 Found 53.21 5.62 18.3

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

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Product Information

Print Date: Mar 11th 2022

Product Name: (±)-5'-Chloro-5'-deoxy-ENBA

CAS Number: 103626-26-2

IUPAC Name: N-Bicyclo[2.2.1]hept-2-yl-5'-chloro-5'-deoxyadenosine

Description:

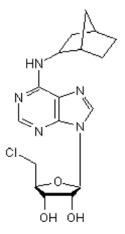
(±)-5'-Chloro-5'-deoxy-ENBA is a highly selective adenosine A₁ receptor agonist (K_i values are 0.51, 1290, 1340 and 2740 nM at A₁, A₃, A_{2A} and A_{2B} receptors respectively). Reverses formalininduced nocifensive behavior in mice; antinociceptive.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₂₂ClN₅O₃.¼H₂O Batch Molecular Weight: 384.34 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Franchetti *et al* (2009) N⁶-cycloalkyl- and N⁶-bicycloalkyl-C5'(C2')-modified adenosine derivatives as high-affinity and selective agonists at the human A₁ adenosine receptor with antinociceptive effects in mice. J.Med.Chem. **52** 2393. PMID: 19317449. **Trivedi** *et al* (1989) N⁶-bicycloalkyladenosines with unusually high potency and selectivity for the adenosine A1 receptor. J.Med.Chem.

Trivedi *et al* (1989) №-bicycloalkyladenosines with unusually high potency and selectivity for the adenosine A1 receptor. J.Med.Chem. **32** 8. PMID: 2909748.

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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.

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