

Certificate of Analysis

Print Date: Aug 8th 2018

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Product Name: Ro 15-4513 Catalog No.: 1997 Batch No.: 5

CAS Number: 91917-65-6

IUPAC Name: 8-Azido-5,6-dihydro-5-methyl-6-oxo-4*H*-imidazo[1,5-*a*][1,4]benzodiazepine-3-carboxylic acid ethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

 $\begin{tabular}{llll} \textbf{Batch Molecular Formula:} & $C_{15}H_{14}N_6O_3$ \\ \textbf{Batch Molecular Weight:} & 326.31 \\ \textbf{Physical Appearance:} & Yellow solid \\ \textbf{Solubility:} & ethanol to 5 mM \\ \end{tabular}$

DMSO to 10 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.45$ (Dichloromethane:Methanol [95:5])

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.21 4.32 25.75 Found 55.36 4.19 25.42

Tel: +44 (0)1235 529449 www.tocris.com/distributors Tel:+1 612 379 2956



Product Information

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IUPAC Name: 8-Azido-5,6-dihydro-5-methyl-6-oxo-4*H*-imidazo[1,5-a][1,4]benzodiazepine-3-carboxylic acid ethyl ester

Description:

High affinity benzodiazepine ligand. K_i values are 3.1 and 5.3 nM for diazepam-insensitive (DI) and diazepam-sensitive (DS) benzodiazepine receptors respectively. Acts as partial inverse agonist at recombinant DS α 1-, α 2-, α 3- and α 5-GABAA receptors. Displays partial agonism at DI α 4- and α 6-GABAA receptors. Antagonizes several behavioral and neurochemical effects of ethanol. Proconvulsant and anxiogenic.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{15}H_{14}N_6O_3$ Batch Molecular Weight: 326.31 Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Desiccate at +4°C

Solubility & Usage Info:

ethanol to 5 mM DMSO to 10 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:

Knoflach *et al* (1996) Pharmacological modulation of the diazepam-insensitive recombinant gamma-aminobutyric acidA receptors alpha 4 beta 2 gamma 2 and alpha 6 beta 2 gamma 2. Mol.Pharmacol. *50* 1253. PMID: 8913357.

Wong and Skolnick (1992) High affinity ligands for 'diazepam-insensitive' benzodiazepine receptors. Eur.J.Pharmacol. **225** 63. PMID: 1311690.

Suzdak et al (1986) A selective imidazobenzodiazepine antagonist of ethanol in the rat. Science 234 1243. PMID: 3022383.