

Certificate of Analysis

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Product Name: CL 218872

Catalog No.: 1709

Batch No.: 2

CAS Number: 66548-69-4

IUPAC Name: 3-Methyl-6-[3-(trifluoromethyl)phenyl]-1,2,4-triazolo[4,3-*b*]pyridazine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₉F₃N₄·½H₂O

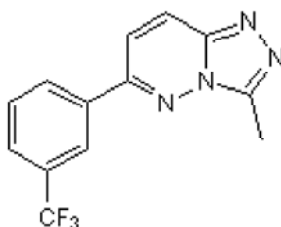
Batch Molecular Weight: 287.25

Physical Appearance: Off White solid

Solubility: DMSO to 50 mM
ethanol to 25 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.36	3.51	19.5
Found	54.64	3.27	19.82

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

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Description:

Benzodiazepine agonist displaying selectivity for α_1 subunit-containing GABA_A receptors (K_i values are 130, 1820, 1530, > 10000, 490 and > 10000 nM for α_1 , α_2 , α_3 , α_4 , α_5 and α_6 -subunit containing receptors respectively). Orally active anxiolytic and anticonvulsant in vivo.

Physical and Chemical Properties:

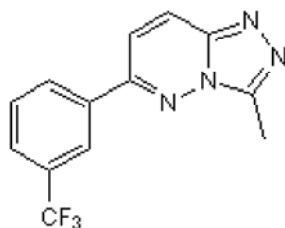
Batch Molecular Formula: C₁₃H₉F₃N₄·½H₂O

Batch Molecular Weight: 287.25

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Sieghart (1995) Structure and pharmacology of γ -aminobutyric acid_A receptor subtypes. *Pharmacol.Rev.* **47** 181. PMID: 7568326.

Lippa et al (1979) Benzodiazepine receptors: cellular and behavioral characteristics. *Pharmacol.Biochem.Behav.* **10** 831. PMID: 40258.

Squires et al (1979) Some properties of brain specific benzodiazepine receptors: new evidence for multiple receptors. *Pharmacol.Biochem.Behav.* **10** 825. PMID: 40257.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 50 mM

ethanol 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.

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