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Certificate of Analysis

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Product Name: Bretazenil

Catalog No.: 3568 Batch No.: 3

CAS Number: IUPAC Name:

(13aS)-8-Bromo-11,12,13,13a-tetrahydro-9-oxo-9H-imidazo[1,5-a]pyrrolo[2,1-c][1,4]benzodiazepine-1-carboxylic acid 1,1-dimethylethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

84379-13-5

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C₁₉H₂₀BrN₃O₃ 418.28 White solid DMSO to 100 mM ethanol to 100 mM Desiccate at +4°C

Storage:

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC:
Chiral HPLC:
¹ H NMR:
Mass Spectrum:
Microanalysis:

Shows 99.6% purity Shows 100% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrog				
Theoretical	54.56	4.82	10.05		
Found	54.33	4.9	9.84		

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

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Description:

IUPAC Name:

Bretazenil is a partial agonist at the GABA_A benzodiazepine site (EC₅₀ = 10 nM at α 1 β 1 γ 2 receptors). Displays anticonvulsive activity in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₂₀BrN₃O₃ Batch Molecular Weight: 418.28 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at +4°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).

Catalog No.: 3568

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Munro *et al* (2008) Comparison of the novel subtype-selective GABAA receptor-positive allosteric modulator NS11394 [3'-[5-(1-hydroxy-1-methyl)-benzoimidazol-1-yl]-biphenyl-2-carbonitrile] with D.pam, zolpidem, bretazenil, and gaboxadol in rat models of i J.Pharmacol.Exp.Ther. **327** 969. PMID: 18791060.

Rundfeldt *et al* (1995) Anticonvulsant tolerance and withdrawal characteristics of benzodiazepine receptor ligands in different seizure models in mice. Comparison of D.pam, bretazenil and abecarnil. J.Pharmacol.Exp.Ther. **275** 693. PMID: 7473156.

Puia *et al* (1992) Molecular mechanisms of the partial allosteric modulatory effects of bretazenil at γ-aminobutyric acid type A receptor. Proc.Natl.Acad.Sci. USA Neurobiology **89** 3620.

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