TOCRIS a biotechne brand

Print Date: Jan 13th 2016

Batch No.: 2

Certificate of Analysis

www.tocris.com

Catalog No.: 1869

Product Name: Ipsapirone

CAS Number: IUPAC Name: 95847-70-4

2-[4-[4-(2-Pyrimidinyl)-1-piperazinyl]butyl]-1,2-benzisothiazol-3(2H)-one-1,1-dioxide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C₁₉H₂₃N₅O₃S 401.48 White solid DMSO to 10 mM Store at RT

2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis: $\label{eq:Rf} \begin{array}{l} \mathsf{R_{f}} = 0.48 \; (\text{Dichloromethane:Methanol} \; [9:1]) \\ \text{Shows } 99.4\% \; \text{purity} \\ \text{Consistent with structure} \\ \text{Consistent with structure} \\ \text{Carbon Hydrogen Nitrogen} \\ \text{Theoretical } 56.84 \quad 5.77 \quad 17.44 \\ \text{Found} \quad 56.95 \quad 5.75 \quad 17.45 \\ \end{array}$

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

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CAS Number: 95847-70-4

2-[4-[4-(2-Pyrimidinyl)-1-piperazinyl]butyl]-1,2-benzisothiazol-3(2H)-one-1,1-dioxide **IUPAC Name:**

Description:

Selective 5-HT_{1A} receptor agonist (K_i = 10 nM). Anxiolytic in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₂₃N₅O₃S Batch Molecular Weight: 401.48 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info: 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).

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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:

Traber et al (1984) Brain serotonin receptors as a target for the putative anxiolytic TVX Q 7821. Brain Res.Bull. 12 741. PMID: 6541079. Glaser and Traber (1985) Binding of the putative anxiolytic TVX Q 7821 to hippocampal 5-hydroxytryptamine (5-HT) recognition sites. Naunyn-Schmied.Arch.Pharmacol. 329 211.

Maj et al (1987) Central action of ipsapirone, a new anxiolytic drug, on serotoninergic, noradrenergic and dopaminergic functions. J.Neural.Transm. 70 1. PMID: 2889795.

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