TOCRIS
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Print Date: Jun 4th 2016

Certificate of Analysis

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Product Name: **GS 39783** **Catalog No.: 2001** **Batch No.: 3**

CAS Number: 39069-52-8

IUPAC Name: *N*,*N*'-Dicyclopentyl-2-(methylthio)-5-nitro-4,6-pyrimidinediamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{23}N_5O_2S$

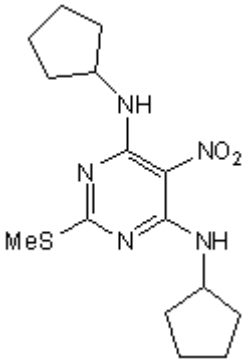
Batch Molecular Weight: 337.44

Physical Appearance: Pale orange solid

Solubility: ethanol to 5 mM
DMSO to 10 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

Melting Point: Between 87 - 89°C

HPLC: Shows 98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.39	6.87	20.74
Found	53.34	6.65	20.63

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Description:

Positive allosteric modulator of $GABA_B$ receptor function. Potentiates the effects of GABA on [^{35}S]GTPγS binding at recombinant and native $GABA_B$ receptors (EC_{50} values are 2.1 and 3.1μM respectively). Decreases cocaine self-administration, blocks the rewarding properties of nicotine and produces anxiolytic-like activity without the side effects associated with baclofen or benzodiazepines.

Physical and Chemical Properties:

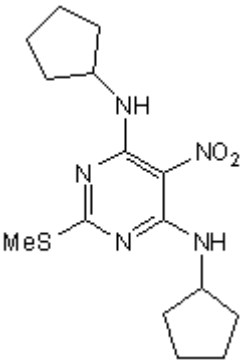
Batch Molecular Formula: $C_{15}H_{23}N_5O_2S$

Batch Molecular Weight: 337.44

Physical Appearance: Pale orange solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

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:

Mombereau *et al* (2007) $GABA_B$ receptor-positive modulation-induced blockade of the rewarding effects of nicotine is associated with a reduction in nucleus accumbens ΔFosB accumulation. J.Pharmacol.Exp.Ther. ***321*** 172. PMID: 17215447.

Cryan *et al* (2004) Behavioral characterization of the novel $GABA_B$ receptor-positive modulator GS39783 (*N,N'*-dicyclopentyl-2-methylsulfanyl-5-nitro-pyrimidine-4,6-diamine: anxiolytic-like activity without side effects associated with baclofen or benzodiazepines. J.Pharmacol.Exp.Ther. ***310*** 952. PMID: 15113848.

Urwyler *et al* (2003) *N,N'*-Dicyclopentyl-2-methylsulfanyl-5-nitro-pyrimidine-4,6-diamine (GS39783) and structurally related compounds: novel allosteric enhancers of γ-aminobutyric $acid_B$ receptor function. J.Pharmacol.Exp.Ther. ***307*** 322. PMID: 12954816.

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