

Product Name: L-838,417

Catalog No.: 3250

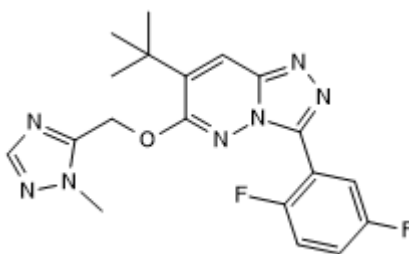
Batch No.: 5

CAS Number: 286456-42-6

IUPAC Name: 3-(2,5-Difluorophenyl)-7-(1,1-dimethylethyl)-6-[(1-methyl-1*H*-1,2,4-triazol-5-yl)methoxy]-1,2,4-triazolo[4,3-*b*]pyridazine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₁₉ H ₁₉ F ₂ N ₇ O·½H ₂ O
Batch Molecular Weight:	403.9
Physical Appearance:	White solid
Solubility:	DMSO to 50 mM ethanol to 20 mM with sonication
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.45 (Chloroform:Methanol [9:1])
HPLC:	Shows 99.7% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	56.5	4.87	24.27
Found	56.71	4.73	24.48

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

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Description:

Subtype-selective GABA_A receptor partial agonist. Selectively binds to $\alpha 1$, $\alpha 2$, $\alpha 3$ and $\alpha 5$ subunits (K_i values are 0.79, 0.67, 0.67 and 2.25 nM respectively) but displays no efficacy at $\alpha 1$ ($\alpha 1$ -sparing). Exhibits non-sedative anxiolytic, antinociceptive and anti-inflammatory activity in vivo.

Physical and Chemical Properties:

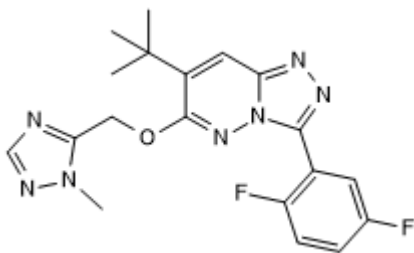
Batch Molecular Formula: C₁₉H₁₉F₂N₇O.¼H₂O

Batch Molecular Weight: 403.9

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 mM

ethanol to 20 mM with sonication

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.

Licensing Information:

Manufactured and sold under license from Merck & Co., Inc. for use solely for preclinical research purposes (ie: not for administration to or other use in humans)

References:

Knabl et al (2008) Reversal of pathological pain through specific spinal GABA_A receptor subtypes. *Nature* **451** 330. PMID: 18202657.

McMahon and France (2006) Differential behavioural effects of low efficacy positive GABA_A modulators in combination with benzodiazepines and a neuroactive steroid in rhesus monkeys. *Br.J.Pharmacol.* **147** 260. PMID: 16331290.

McCabe et al (2004) Subtype-selective GABAergic drugs facilitate extinction of mouse operant behaviour. *Neuropharmacology* **46** 171. PMID: 14680756.

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