

Product Name: MRK 016

Catalog No.: 3817

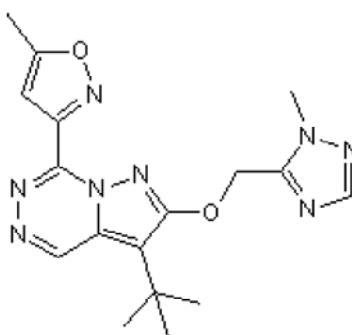
Batch No.: 4

CAS Number: 342652-67-9

IUPAC Name: 3-(1,1-Dimethylethyl)-7-(5-methyl-3-isoxazolyl)-2-[(1-methyl-1*H*-1,2,4-triazol-5-yl)methoxy]-pyrazolo[1,5-*d*][1,2,4]triazine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₀N₈O₂
Batch Molecular Weight: 368.39
Physical Appearance: White solid
Solubility: DMSO to 50 mM
 ethanol to 20 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.43	5.47	30.42
Found	55.33	5.49	30.2

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

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Description:

GABA_A receptor inverse agonist selective for the α5-subtype (EC₅₀ = 3 nM). Exhibits affinity at benzodiazepine binding site of recombinant human GABA_A receptors (K_i values are 0.77 nM, 0.83 nM, 0.85 nM and 1.4 nM for α3-, α1-, α2-, and α5-containing respectively). Increases long-term potentiation (LTP) in mouse hippocampal slices. Exhibits no anxiogenic or proconvulsant activity.

Physical and Chemical Properties:

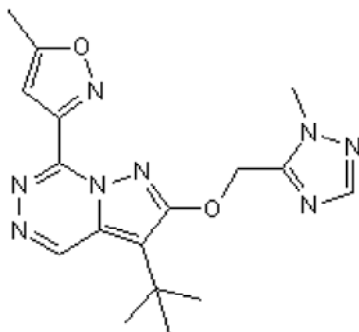
Batch Molecular Formula: C₁₇H₂₀N₈O₂

Batch Molecular Weight: 368.39

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Atack et al (2009) In vitro and in vivo properties of 3-tert-butyl-7-(5-methylisoxazol-3-yl)-2-(1-methyl-1*H*-1,2,4-triazol-5-ylmethoxy)-pyrazolo[1,5-*d*]-[1,2,4]triazine (MRK-016), a GABA_A receptor α5 subtype-selective inverse agonist. *J.Pharmacol.Exp.Ther.* **331** 470. PMID: 19704033.

Chambers et al (2004) An orally bioavailable, functionally selective inverse agonist at the benzodiazepine site of GABA_A α5 receptors with cognition enhancing properties. *J.Med.Chem.* **47** 5829. PMID: 15537339.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 mM

ethanol to 20 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.

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)

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