

Product Name: Ro 61-8048

Catalog No.: 3254

Batch No.: 8

CAS Number: 199666-03-0

IUPAC Name: 3,4-Dimethoxy-N-[4-(3-nitrophenyl)-2-thiazolyl]benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₅N₃O₆S₂·½H₂O

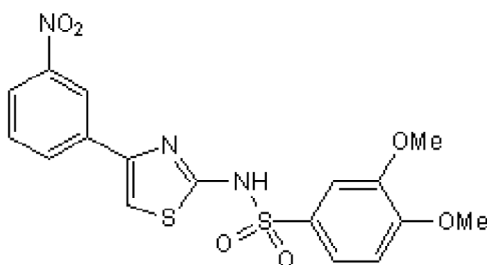
Batch Molecular Weight: 425.95

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 10 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.94	3.67	9.86
Found	47.38	3.45	9.68

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

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CAS Number: 199666-03-0

IUPAC Name: 3,4-Dimethoxy-N-[4-(3-nitrophenyl)-2-thiazolyl]benzenesulfonamide

Description:

Ro 61-8048 is a potent and competitive kynurenine 3-monooxygenase (kynurenine 3-hydroxylase; KMO) inhibitor ($K_i = 4.8$ nM, $IC_{50} = 37$ nM). Increases kynurenic acid levels to concentrations that antagonize the glycine site of NMDA receptors. Brain penetrant and exhibits antidystonic, anticonvulsant and neuroprotective activities. Ro 61-8048 decreases nicotine self-administration in vivo. Ro 61-8048 prevents post-operative brain edema and consequent neuronal apoptosis in a rat model of surgically induced brain injury.

Physical and Chemical Properties:

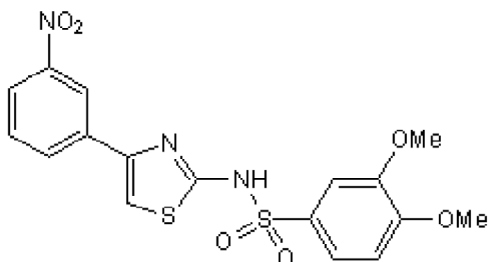
Batch Molecular Formula: $C_{17}H_{15}N_3O_6S_2 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 425.95

Physical Appearance: Yellow solid

Minimum Purity: $\geq 99\%$

Batch Molecular Structure:



References:

Zakhary *et al* (2020) Modification of kynurenine pathway via inhibition of kynurenine hydroxylase attenuates surgical brain injury complications in a male rat model. *J Neurosci Res* **98** 155. PMID: 31257634.

Secci *et al* (2017) Attenuating nicotine reinforcement and relapse by enhancing endogenous brain levels of kynurenic acid in rats and squirrel monkeys. *Neuropsychopharmacology* **42** 1619. PMID: 28139681.

Justinova *et al* (2013) Reducing cannabinoid abuse and preventing relapse by enhancing endogenous brain levels of kynurenic acid. *Nat. Neurosci.* **16** 1652. PMID: 24121737.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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. *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.

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