

Product Name: Ro 61-8048

Catalog No.: 3254

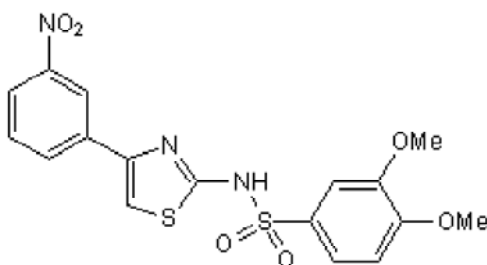
Batch No.: 5

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
Batch Molecular Weight: 421.45
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 100.0% purity
¹H NMR: consistent with structure
Mass Spectrum: consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.45	3.59	9.97
Found	48.05	3.61	9.85

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

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Description:

Potent and competitive kynurenine 3-monoxygenase (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.

Physical and Chemical Properties:

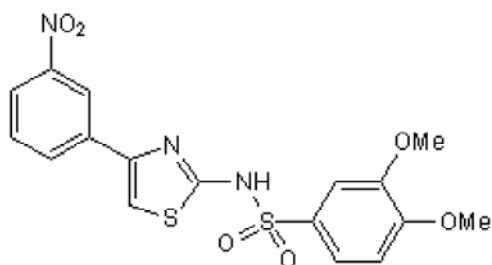
Batch Molecular Formula: C₁₇H₁₅N₃O₆S₂

Batch Molecular Weight: 421.45

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

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

Hamann et al (2008) Effects of kynurenine 3-hydroxylase inhibitor Ro 61-8048 after intrastriatal injections on the severity of dystonia in the *dt^{sz}* mutant. *Eur.J.Pharmacol.* **586** 156. PMID: 18353306.

Carpenido et al (2002) Kynurenine 3-mono-oxygenase inhibitors attenuate post-ischaemic neuronal death in organotypic hippocampal slice cultures. *J.Neurochem.* **82** 1465. PMID: 12354294.

Rover et al (1997) Synthesis and biochemical evaluation of *N*-(4-phenylthiazol-2-yl)benzenesulfonamides as high affinity inhibitors of kynurenine 3-hydroxylase. *J.Med.Chem.* **40** 4378. PMID: 9435907.

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. 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.

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