

Certificate of Analysis

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Product Name: Ro 67-7476

Catalog No.: 4346

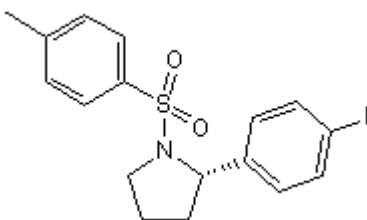
Batch No.: 1

CAS Number: 298690-60-5

IUPAC Name: (2S)-2-(4-Fluorophenyl)-1-[(4-methylphenyl)sulfonyl]-pyrrolidine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₈FNO₂S
Batch Molecular Weight: 319.39
Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.51 (Ethyl acetate:Petroleum ether [2:3])
HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -175 (Concentration = 1, Solvent = Chloroform)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.93	5.68	4.39
Found	63.56	5.44	4.43

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

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Description:

Positive allosteric modulator of mGlu₁ receptors. Potentiates glutamate-induced calcium release (EC₅₀ = 60.1 nM at rat mGluR1a). Displays no activity at human mGlu₁ receptors.

Physical and Chemical Properties:

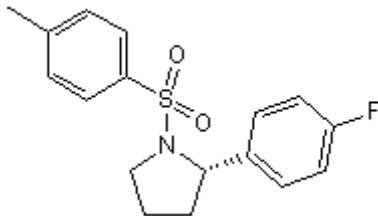
Batch Molecular Formula: C₁₇H₁₈FNO₂S

Batch Molecular Weight: 319.39

Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Knoflach et al (2001) Positive allosteric modulators of metabotropic glutamate 1 receptor: characterization, mechanism of action, and binding site. *Proc.Natl.Acad.Sci.USA* **98** 13402. PMID: 11606768.

Hemstapat et al (2006) A novel class of positive allosteric modulators of metabotropic glutamate receptor subtype 1 interact with a site distinct from that of negative allosteric modulators. *Mol.Pharmacol.* **70** 616. PMID: 16645124.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 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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