

Product Name: SB 674042

Catalog No.: 4673

Batch No.: 1

CAS Number: 483313-22-0

IUPAC Name: [5-(2-Fluorophenyl)-2-methyl-4-thiazolyl][2(S)-2-[(5-phenyl-1,3,4-oxadiazol-2-yl)methyl-1-pyrrolidiny]]methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₁FN₄O₂S.½H₂O

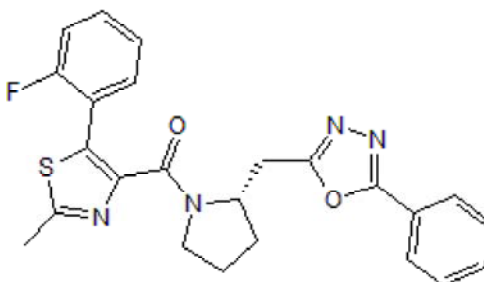
Batch Molecular Weight: 457.52

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.59 (Chloroform:Methanol [9:1])

HPLC: Shows 97.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -65.5 (Concentration = 1, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.01	4.85	12.25
Found	63.11	4.71	12.32

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

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Description:

Potent and selective non-peptide orexin OX₁ receptor antagonist (K_d = 3.76 nM). Exhibits 100-fold selectivity for OX₁ over OX₂ receptors. Has no effect at serotonergic, dopaminergic, adrenergic or purinergic receptors. Inhibits orexin 1-induced Ca²⁺ mobilization in CHO-DG44 cells stably transfected with the OX₁ receptor.

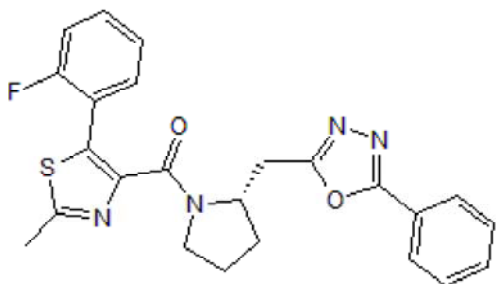
Physical and Chemical Properties:

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References:

Ellis et al (2006) Orexin-1 receptor-cannabinoid CB1 receptor heterodimerization results in both ligand-dependent and -independent coordinated alterations of receptor localization and function. *Biol.Chem.* **281** 38812. PMID: 17015451.

Langmead et al (2004) Characterisation of the binding of [3H]-SB-674042, a novel nonpeptide antagonist, to the human orexin-1 receptor. *Br.J.Pharmacol.* **141** 340. PMID: 14691055.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

Licensing Information:

Sold for research purposes under agreement from GlaxoSmithKline.

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