

Product Name: TCS 1102

Catalog No.: 3818

Batch No.: 2

CAS Number: 916141-36-1

IUPAC Name: *N*-[1,1'-Biphenyl]-2-yl-1-[2-[(1-methyl-1*H*-benzimidazol-2-yl)thio]acetyl]-2-pyrrolidinedicarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₂₆N₄O₂S·¼H₂O

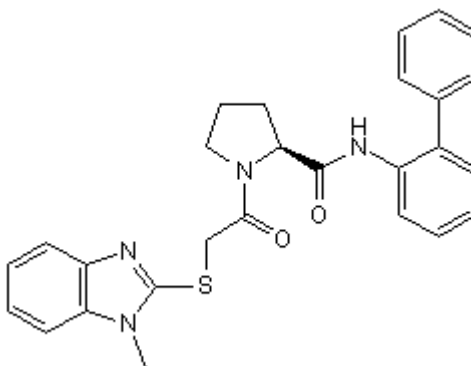
Batch Molecular Weight: 475.09

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Ethyl acetate:Petroleum ether [9:1])

HPLC: Shows >98.4% purity

Chiral HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.26	5.62	11.79
Found	68.09	5.66	11.55

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

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Description:

Potent, dual orexin receptor antagonist (K_i values are 0.2 and 3 nM for OX_2 and OX_1 receptors respectively). Inhibits ADL-orexin B-mediated locomotion following i.p. administration in vivo and blocks orexin-A (Cat.No.1455) mediated increases in feeding behaviour. Brain penetrant.

Physical and Chemical Properties:

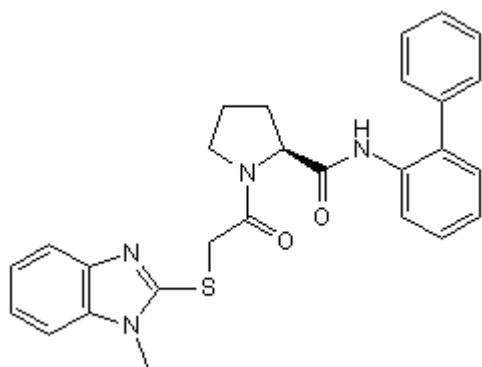
Batch Molecular Formula: $C_{27}H_{26}N_4O_2S \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 475.09

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

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:

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)

References:

Khoo et al (2017) The dual orexin receptor antagonist TCS1102 does not affect reinstatement of nicotine-seeking. *PLoS One* **12**. PMID: 28296947.

Winrow et al (2010) Orexin receptor antagonism prevents transcriptional and behavioral plasticity resulting from stimulant exposure. *Neuropharmacology* **58** 185. PMID: 19596018.

Bergman et al (2008) Proline bis-amides as potent dual orexin receptor antagonists. *Bioorg.Med.Chem.Letts* **18** 1425.

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