

**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:** C<sub>27</sub>H<sub>26</sub>N<sub>4</sub>O<sub>2</sub>S·¼H<sub>2</sub>O

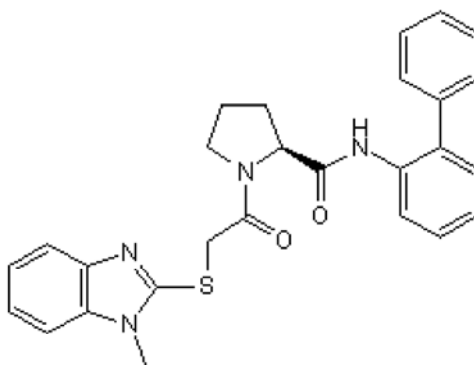
**Batch Molecular Weight:** 475.09

**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<sub>f</sub> = 0.25 (Ethyl acetate:Petroleum ether [9:1])

**HPLC:** Shows 98.4% purity

**Chiral HPLC:** Shows 98.6% purity

**<sup>1</sup>H 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

**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel:+1 612 379 2956

**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

**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:**

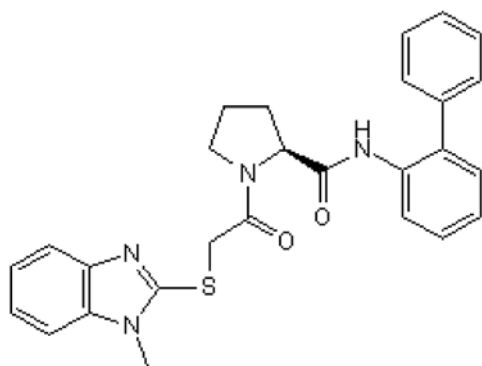
Batch Molecular Formula:  $C_{27}H_{26}N_4O_2S \cdot \frac{1}{4}H_2O$

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** e0173967. 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.

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

**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel:+1 612 379 2956