

**Product Name:** TCS OX2 29

**Catalog No.:** 3371

**Batch No.:** 2

CAS Number: 372523-75-6

IUPAC Name: (2S)-1-(3,4-Dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)-3,3-dimethyl-2-[(4-pyridinylmethyl)amino]-1-butanone hydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>23</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>·HCl·3H<sub>2</sub>O

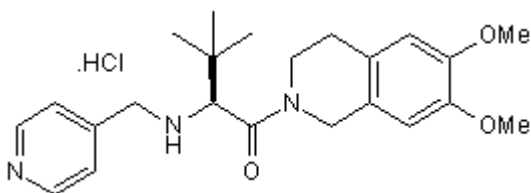
**Batch Molecular Weight:** 488.02

**Physical Appearance:** Pale yellow solid

**Solubility:** water to 100 mM  
DMSO to 25 mM  
ethanol to 5 mM

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 98.3% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = +48 (Concentration = 1, Solvent = Water)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	56.61	7.85	8.61
Found	56.61	7.36	8.65

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

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**Description:**

Potent and selective OX<sub>2</sub> receptor antagonist (IC<sub>50</sub> = 40 nM). Displays >250-fold selectivity for OX<sub>2</sub> over OX<sub>1</sub> and a range of receptors, ion channels and transporters. Inhibits orexin A induced IP<sub>3</sub> accumulation and ERK1/2 phosphorylation in CHO cells transfected with the OX<sub>2</sub> receptor.

**Physical and Chemical Properties:**

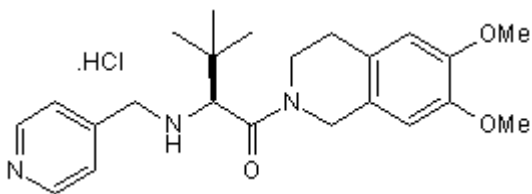
Batch Molecular Formula: C<sub>23</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>.HCl.3H<sub>2</sub>O

Batch Molecular Weight: 488.02

Physical Appearance: Pale yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Mould et al** (2014) Binding kinetics differentiates functional antagonism of orexin-2 receptor ligands. *Br.J.Pharmacol.* **171** 351. PMID: 23692283.

**Hirose et al** (2003) *N*-acyl 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline: The first orexin-2 receptor selective non-peptidic antagonist. *Bioorg.Med.Chem.Lett.* **13** 4497. PMID: 14643355.

**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**

water to 100 mM

DMSO to 25 mM

ethanol to 5 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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