

**Certificate of Analysis** 

www.tocris.com

Print Date: Jan 14th 2016

Product Name: PTAC oxalate Catalog No.: 4533 Batch No.: 1

CAS Number: 201939-40-4

IUPAC Name: (1R,5R,6R)-6-[4-(Propylthio)-1,2,5-thiadiazol-3-yl]-1-azabicyclo[3.2.1]octane oxalate

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{12}H_{19}N_3S_2.C_2H_2O_4$ 

**Batch Molecular Weight:** 359.46 **Physical Appearance:** White solid

**Solubility:** water to 100 mM

DMSO to 100 mM ethanol to 100 mM

Storage: Desiccate at RT

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.65$  (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows 100% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

**Optical Rotation:**  $[\alpha]_D = -5$  (Concentration = 0.2, Solvent = Methanol)



# **Product Information**

Print Date: Jan 14th 2016

www.tocris.com

Product Name: PTAC oxalate Catalog No.: 4533 Batch No.: 1

CAS Number: 201939-40-4

IUPAC Name: (1R,5R,6R)-6-[4-(Propylthio)-1,2,5-thiadiazol-3-yl]-1-azabicyclo[3.2.1]octane oxalate

#### **Description:**

Muscarinic receptor ligand. Displays partial agonist activity at  $M_2$  and  $M_4$  receptors; exhibits antagonist effects at  $M_1,\ M_3$  and  $M_5$  receptors ( $K_i$  values are 2.8, 0.2, 0.6, 0.2 and 0.8 nM respectively). Displays selectivity for muscarinic receptors over a range of neurotransmitter receptors and ion channels. Inhibits firing rate of dopaminergic cells in the limbic ventral tegmental area after acute administration, without binding to dopamine receptors.

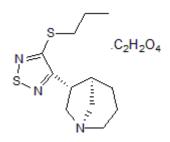
#### **Physical and Chemical Properties:**

Batch Molecular Formula:  $C_{12}H_{19}N_3S_2.C_2H_2O_4$ 

Batch Molecular Weight: 359.46 Physical Appearance: White solid

**Minimum Purity:** >98%

#### **Batch Molecular Structure:**



Storage: Desiccate at RT

### Solubility & Usage Info:

water to 100 mM 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.

## References:

**Bymaster** *et al* (1998) Unexpected antipsychotic-like activity with the muscarinic receptor ligand (5*R*,6*R*)6-(3-propylthio-1,2,5-thiadiazol-4-yl)-1-azabicyclo[3.2.1]octane. Eur.J.Pharmacol. *356* 109. PMID: 9774240.

**Shannon** *et al* (1999) Muscarinic receptor agonists, like dopamine receptor antagonist antipsychotics, inhibit conditioned avoidance response in rats. J.Pharmacol.Exp.Ther. **290** 901. PMID: 10411607.

Raedler et al (2007) Towards a muscarinic hypothesis of schizophrenia. Mol.Psychiatry 12 232. PMID: 17146471.