bio-techne
TOCRIS

Print Date: Jul 26th 2023

Certificate of Analysis

www.tocris.com

Product Name: **Xanomeline oxalate** **Catalog No.: 3569** **Batch No.: 4**

CAS Number: 141064-23-5

IUPAC Name: 3-[4-(Hexyloxy)-1,2,5-thiadiazol-3-yl]-1,2,5,6-tetrahydro-1-methylpyridine oxalate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_{23}N_3OS.C_2H_2O_4$

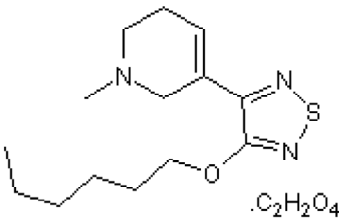
Batch Molecular Weight: 371.46

Physical Appearance: Off White solid

Solubility: water to 10 mM with gentle warming
DMSO to 100 mM
ethanol to 25 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.74	6.78	11.31
Found	51.67	6.78	11.14

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Description:

Xanomeline oxalate is a functionally biased muscarinic M_4 receptor agonist (EC_{50} values are 14.1 nM, 30.9 nM, 1700 nM, 1800 nM and 8500 nM at M_4, M_1, M_2, M_5 and M_3 receptors respectively. Binds with similar affinity to all muscarinic acetylcholine receptors (pKi 6.7-7.7) but displays higher efficacy and efficacy-driven selectivity at M_4 receptors. Displays a complex pharmacological profile: reversible and wash-resistant binding, resulting in full agonist activity at M_1; delayed wash-resistant partial agonist activity at M_2; and delayed wash-resistant full agonist activity at M_4. Exhibits antipsychotic activity, and improves cognitive deficits... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

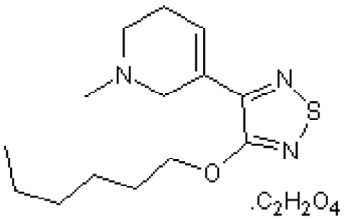
Batch Molecular Formula: $C_{14}H_{23}N_3OS.C_2H_2O_4$

Batch Molecular Weight: 371.46

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 10 mM with gentle warming
DMSO to 100 mM
ethanol to 25 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Heinrich *et al* (2009) Pharmacological comparison of muscarinic ligands: historical versus more recent muscarinic M_1-preferring receptor agonists. Eur.J.Pharmacol. ***605*** 53. PMID: 19168056.

Jakubik *et al* (2008) Importance and prospects for design of selective muscarinic agonists. Physiol.Res. ***57*** S39. PMID: 18481916.

Stanhope *et al* (2001) The muscarinic receptor agonist xanomeline has an antipsychotic-like profile in the rat. J.Pharmacol.Exp.Ther. ***299*** 782. PMID: 11602695.