

Product Name: Xanomeline oxalate

Catalog No.: 3569

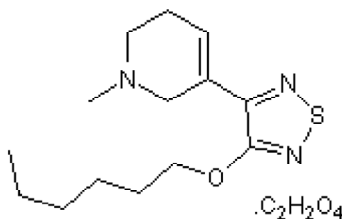
Batch No.: 5

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: C₁₄H₂₃N₃OS.C₂H₂O₄.
Batch Molecular Weight: 371.46
Physical Appearance: White solid
Solubility: water to 10 mM with gentle warming
DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.74	6.78	11.31
Found	51.98	6.72	11.44

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

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Description:

Xanomeline oxalate is a functionally biased muscarinic M₄ receptor agonist (EC₅₀ values are 14.1 nM, 30.9 nM, 1700 nM, 1800 nM and 8500 nM at M₄, M₁, M₂, M₅ and M₃ receptors respectively. Binds with similar affinity to all muscarinic acetylcholine receptors (pK_i 6.7-7.7) but displays higher efficacy and efficacy-driven selectivity at M₄ receptors. Displays a complex pharmacological profile: reversible and wash-resistant binding, resulting in full agonist activity at M₁; delayed wash-resistant partial agonist activity at M₂; and delayed wash-resistant full agonist activity at M₄. Exhibits antipsychotic activity, and improves cognitive deficits... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

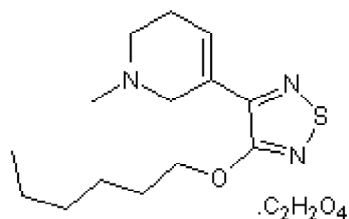
Batch Molecular Formula: C₁₄H₂₃N₃OS.C₂H₂O₄.

Batch Molecular Weight: 371.46

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Powers et al (2023) Structural basis of efficacy-driven ligand selectivity at GPCRs. *Nat.Chem.Biol.* **19** 805. PMID: 36782010.

McDonald et al (2022) Biased profile of xanomeline at the recombinant human M₄ muscarinic acetylcholine receptor. *ACS Chem.Neurosci.* **13** 1206. PMID: 35380782.

Heinrich et al (2009) Pharmacological comparison of muscarinic ligands: historical versus more recent muscarinic M₁-preferring receptor agonists. *Eur.J.Pharmacol.* **605** 53. PMID: 19168056.

Storage: Store at +4°C

Solubility & Usage Info:

water to 10 mM with gentle warming
DMSO 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. *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.

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