TOCRIS
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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **ML 277** **Catalog No.: 4777** **Batch No.: 1**

CAS Number: 1401242-74-7

IUPAC Name: (2*R*)-*N*-[4-(4-Methoxyphenyl)-2-thiazolyl]-1-[(4-methylphenyl)sulfonyl]-2-piperidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{25}N_3O_4S_2 \cdot ¼H_2O$

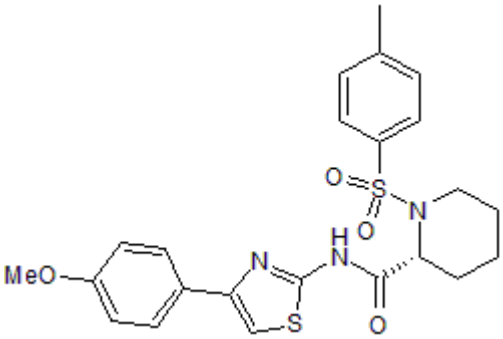
Batch Molecular Weight: 476.09

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.59 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 100% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +67.5 (Concentration = 1, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.03	5.4	8.83
Found	58.1	5.31	8.74

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Description:

Selective $K_v7.1$ (KCNQ1) potassium channel activator (EC_{50} = 260 nM). Exhibits >100-fold selectivity versus KCNQ2, KCNQ4 and hERG potassium channels. Augments I_{Ks} current of cultured human cardiomyocytes and shortens action potential duration.

Physical and Chemical Properties:

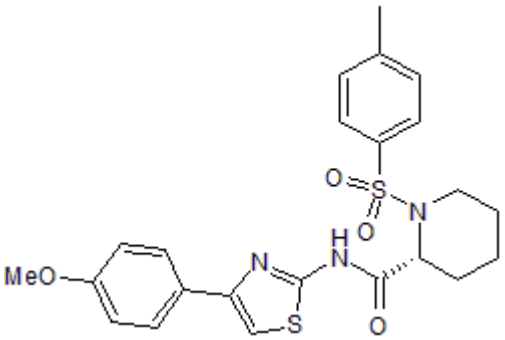
Batch Molecular Formula: $C_{23}H_{25}N_3O_4S_2.¼H_2O$

Batch Molecular Weight: 476.09

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

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. 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:

Mattmann *et al* (2012) Identification of (*R*)-*N*-(4-(4-methoxyphenyl)thiazol-2-yl)-1-tosylpiperidine-2-carboxamide, ML277, as a novel, potent and selective $K_v7.1$ (KCNQ1) potassium channel activator. Bioorg.Med.Chem.Lett. ***22*** 5936. PMID: 22910039.

Yu *et al* (213) Dynamic subunit stoichiometry confers a progressive continuum of pharmacological sensitivity by KCNQ potassium channels. Proc.Natl.Acad.Sci.U.S.A. ***110*** 8732. PMID: 23650380.

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