TOCRIS
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Print Date: Jun 6th 2019

# Certificate of Analysis

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**Product Name:** **ML 335** **Catalog No.: 6887** **Batch No.: 1**

CAS Number: 825658-06-8

IUPAC Name: *N*-[(2,4-Dichlorophenyl)methyl]-4-[(methylsulfonyl)amino]benzamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{15}H_{14}Cl_2N_2O_3S$

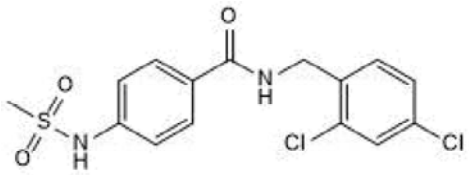
**Batch Molecular Weight:** 373.25

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM
ethanol to 20 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.22 (Ethyl acetate:Petroleum ether [1:1])

**HPLC:** Shows 99.1% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 48.27 | 3.78 | 7.51 |
| Found | 48.2 | 3.75 | 7.48 |



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IUPAC Name: *N*-[(2,4-Dichlorophenyl)methyl]-4-[(methylsulfonyl)amino]benzamide

**Description:**

Selective $K_{2P}2.1$ (TREK-1; KCNK2) and $K_{2P}10.1$ (TREK-2; KCNK10) activator ($EC_{50}$ values of 14.3 µM and 5.2 µM, respectively); directly stimulates the C-type gate via the $K_{2P}$ modulator pocket. Does not activate $K_{2P}4.1$ (TRAAK).

**Physical and Chemical Properties:**

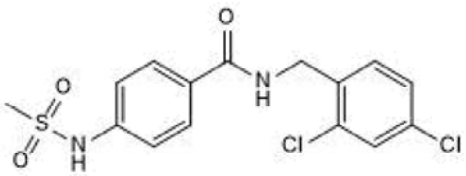
Batch Molecular Formula: $C_{15}H_{14}Cl_2N_2O_3S$

Batch Molecular Weight: 373.25

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM
ethanol to 20 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:**

**Gada** *et al* (2019) Two-pore domain potassium channels: emerging targets for novel analgesic drugs: IUPHAR Review 26. Br.J.Pharmacol. ***176*** 256. PMID: 30325008.

**Schewe** *et al* (2019) A pharmacological master key mechanism that unlocks the selectivity filter gate in $K^+$ channels. Science ***363*** 875. PMID: 30792303.

**Pope** *et al* (2018) Protein and chemical determinants of BL-1249 action and selectivity for $K_{2P}$ channels. ACS Chem.Neurosci. ***9*** 3153. PMID: 30089357.

**Lolicato** *et al* (2017) $K_{2P}2.1$ (TREK-1)-activator complexes reveal a cryptic selectivity filter binding site. Nature ***547*** 364. PMID: 28693035.



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