

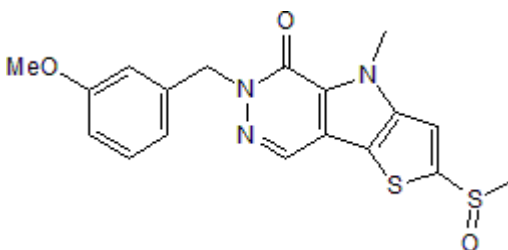
## Certificate of Analysis

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**Product Name:** ML 202 **Catalog No.:** 4859 **Batch No.:** 1  
**CAS Number:** 1221186-52-2  
**IUPAC Name:** 4,6-Dihydro-6-[(3-methoxyphenyl)methyl]-4-methyl-2-(methylsulfinyl)-5H-thieno[2',3':4,5]pyrrolo[2,3-d]pyridazin-5-one

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>18</sub>H<sub>17</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>  
**Batch Molecular Weight:** 387.48  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.43 (Dichloromethane:Methanol [95:5])  
**HPLC:** Shows >98.5% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	55.8	4.42	10.84
Found	55.46	4.43	10.7

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**Description:**

Potent activator of pyruvate kinase M2 (PKM2) ( $IC_{50} = 73$  nM). Exhibits little or no activity against the pyruvate kinase isozymes PKM1, PKL and PKR.

**Physical and Chemical Properties:**

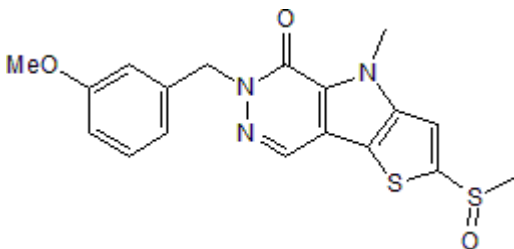
Batch Molecular Formula:  $C_{18}H_{17}N_3O_3S_2$

Batch Molecular Weight: 387.48

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°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:**

**Boxer et al** (2010) Identification of activators for the M2 isoform of human pyruvate kinase version 3. Probe Reports from the Molecular Libraries Program. PMID: 21735594.

**Jiang et al** (2010) Evaluation of thieno[3,2-*b*]pyrrolo[3,2-*d*]pyridazinones as activators of the tumor cell specific M2 isoform of pyruvate kinase. *Bioorg.Med.Chem.Lett.* **20** 3387. PMID: 20451379.

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